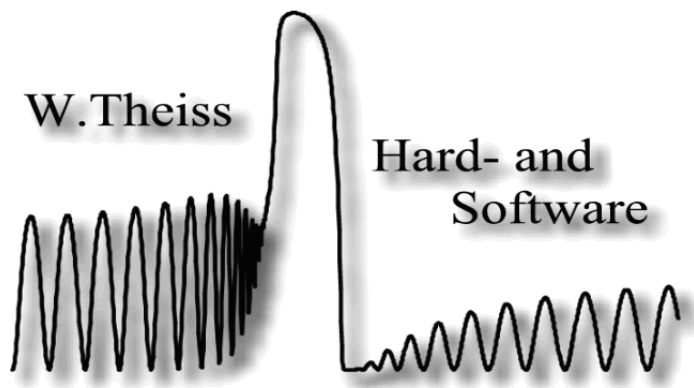


GenetiCode



W.Theiss Hard- and Software for Optical Spectroscopy
Dr.-Bernhard-Klein-Str. 110, D-52078 Aachen
Phone: (49) 241 5661390 Fax: (49) 241 9529100
E-mail: theiss@mtheiss.com Web: www.mtheiss.com



GenetiCode

Optical coating design by genetic algorithms

by Wolfgang Theiss

All rights reserved. No parts of this work may be reproduced in any form or by any means - graphic, electronic, or mechanical, including photocopying, recording, taping, or information storage and retrieval systems - without the written permission of the publisher.

Products that are referred to in this document may be either trademarks and/or registered trademarks of the respective owners. The publisher and the author make no claim to these trademarks.

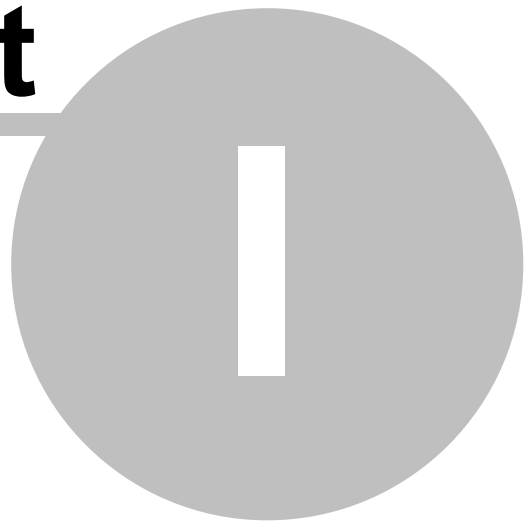
While every precaution has been taken in the preparation of this document, the publisher and the author assume no responsibility for errors or omissions, or for damages resulting from the use of information contained in this document or from the use of programs and source code that may accompany it. In no event shall the publisher and the author be liable for any loss of profit or any other commercial damage caused or alleged to have been caused directly or indirectly by this document.

Printed: 2/15/2019, 4:18 PM in Aachen, Germany

Table of Contents

Foreword	0
Part I Overview	2
1 About this document	3
2 GenetiCode overview	4
3 Installation	5
4 About the author	5
Part II A first application example	6
1 Step-by-step example: A simple anti-reflection coating	7
2 Step 1: Definition of the available materials	8
3 Step 2: Deposition steps	9
4 Step 3: Algorithm parameters	10
5 Step 4: Automatic design	11
6 Step 5: Inspection of the results	12
Part III A three-layer anti-reflection coating	15
1 Modifications of the first example	16
2 Results	18
Part IV 'Invention' of low-E coatings	22
1 Three layer coating	23
2 Five layer coating	25
Part V Optical filters	28
1 Edge filters	29
2 Bandpass filters	35
Part VI Master parameters	39
Index	0

Part



1 Overview

1.1 About this document



Coating design by genetic algorithms

written by W.Theiss

W. Theiss – Hard- and Software for Optical Spectroscopy
Dr.-Bernhard-Klein-Str. 110, D-52078 Aachen, Germany
Phone: + 49 241 5661390 Fax: + 49 241 9529100
e-mail: theiss@mtheiss.com web: www.mtheiss.com

February 2019

1.2 GenetiCode overview

GenetiCode is a Windows 7/8/10 application that designs optical coatings using a genetic algorithm. The user describes the deposition capabilities and the wanted optical properties of the coating. *GenetiCode* tries to achieve the best design selecting appropriate materials and layer thicknesses.

Description of the deposition steps

GenetiCode's structure reflects the following situation: Your coating equipment deposits coatings in well-defined steps, i.e. you are using a sequence of sputtering devices or various subsequent runs in a batch coater. For each basic deposition step there is a list of possible materials. The optical constants of the produced materials and the available thickness range must be known. The number of deposition steps and the possible materials for each step define the deposition equipment that *GenetiCode* will use in order to find the best coating design.

Definition of the optimization target

CODE (Coating Designer), a thin film design software by W.Theiss Hard- and Software, is the heart of *GenetiCode*. Internally *GenetiCode* works with a CODE configuration in order to define the target of the optimization. In CODE you can specify spectra like transmittance or reflectance that are computed based on the coating design. For each spectrum you can enter a target spectrum that *GenetiCode* tries to reach in the optimization procedure. On the other hand, you can also optimize technical data like color coordinates or integral reflectance or transmittance values. The so-called fit deviation in CODE is used by *GenetiCode* in order to quantify the quality of a coating. The lower the fit deviation in CODE the higher the 'fitness' of a design in *GenetiCode*.

CODE offers master parameters which can be introduced to set values of model parameters by user-defined expressions. This mechanism can be used to implement relations between parameters. With master parameters you can, for example, let parameter A always be 3 times as large as parameter B, or you can adapt coating properties (thickness, optical constants) to temperature changes. Starting with GenetiCode version 1.4 you can optimize CODE master parameters in addition to thickness values and material selection as described above.

Controlling the genetic algorithm

GenetiCode uses a genetic algorithm to optimize the coating design. It works like this: Initially a certain number of coatings (each one is a particular choice of a material and a thickness for each deposition step) are chosen randomly. This number is called population. For each coating the fitness is computed. Then new generations are created by the birth of two child coatings from two parent coatings. The selection of the parents is controlled by their fitness, in the sense that the fittest have a larger probability for getting children than the less fitter ones. During the transition from one generation to the next parent genes (i.e. thickness and material information) are eventually exchanged such that the child's genes are a mixture of the parent properties. This gene exchange is controlled by the so-called crossover probability. In addition, a gene may be randomly modified from one to the next generation. The probability for this event is called mutation probability. Since genetic algorithms are games based on a lot of random numbers you should not hope that you find a good (or even the best) solution in each attempt. It is recommended that you try several 'evolution runs' which can be done easily in *GenetiCode*.

Getting started

In order to use *GenetiCode* you must be familiar with CODE. Experienced CODE users will be able to handle *GenetiCode* in a few hours. The easiest way is to follow the introductory step-by-step examples. Before you do that you have to install *GenetiCode* which is described in the next section.

1.3 Installation

The installation of *GenetiCode* is quite simple: Just copy all delivered files to your CODE directory. If you like you can create a shortcut to the program file `geneticode.exe` on your desktop and in your Start menu. You must have purchased and installed CODE in order to work with *GenetiCode*.

The following files are to be copied:

geneticode.exe	the program
geneticode_passport.wtp	the passport file
geneticode.pdf	this document in PDF format for easy printing
start.gcd	start configuration
AR_Si_3layers.gcd	configuration of the second example
Low_E_3layers.gcd	start configuration for the low-E example
Low_E_5layers.gcd	configuration of the 5 layers low-E example
edge_on_glass_superlattice.gcd	edge filter configuration
band_pass_on_glass.gcd	bandpass filter configuration

1.4 About the author

Responsible for all good and bad program features:

Wolfgang Theiss
WTheiss Hardware and Software
11875 E Elin Ranch Road
Tucson, AZ 85749
USA

Phone: (1) 928 985 0821
e-mail: theiss@mttheiss.com
Web: wtheiss.com

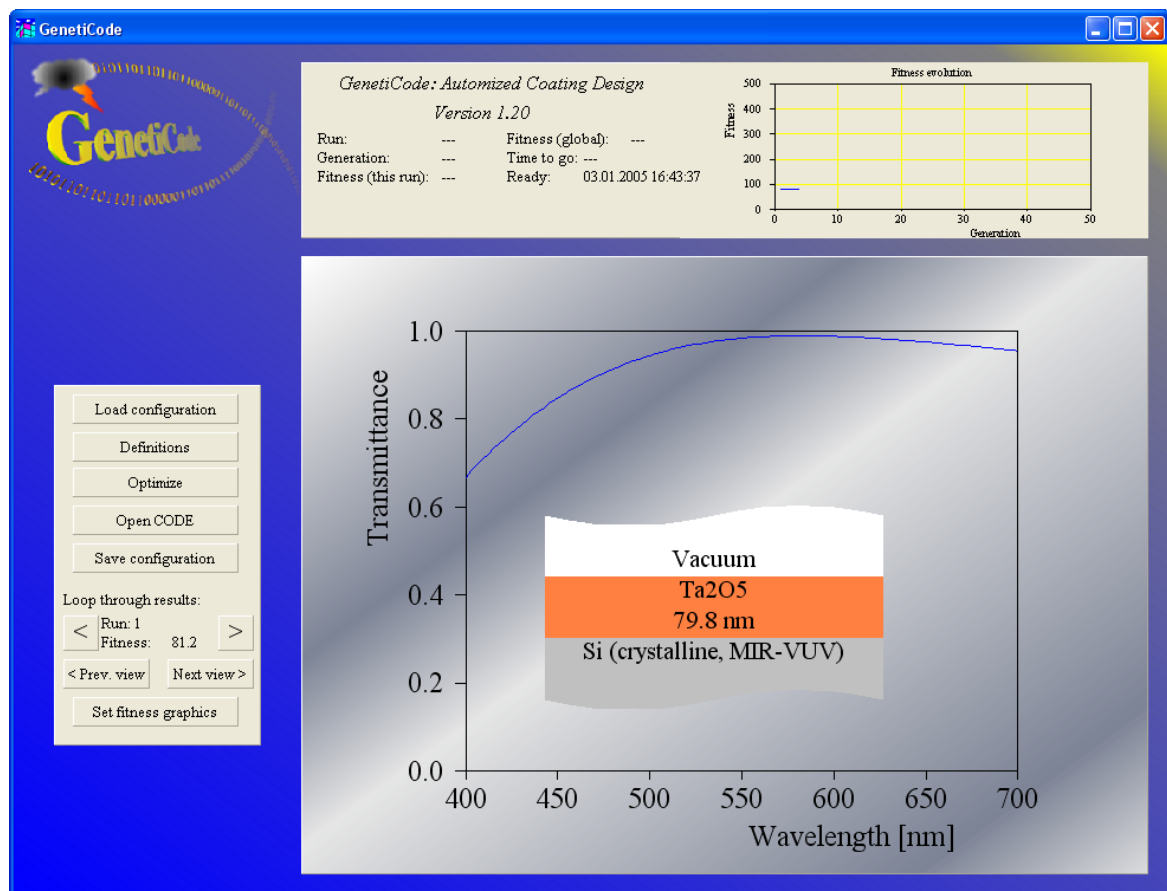
Part



2 A first application example

2.1 Step-by-step example: A simple anti-reflection coating

In order to demonstrate and explain the basic features of *GenetiCode* we use a very simple design problem. For a silicon detector we want to optimize the light transmission from air to silicon by an additional layer. At normal incidence of light the reflectance of the air-silicon interface is higher than 30% in the visible. Hence the transmission is below 70% which is going to be increased by an appropriate anti-reflection layer. *GenetiCode* is used to find out the right material and layer thickness. If you start *GenetiCode* it searches in its directory for the starting configuration start.gcd and loads it. This configuration is prepared for this first application example. If you have turned into an advanced user you can overwrite this file by the start configuration of your choice. The following window appears:

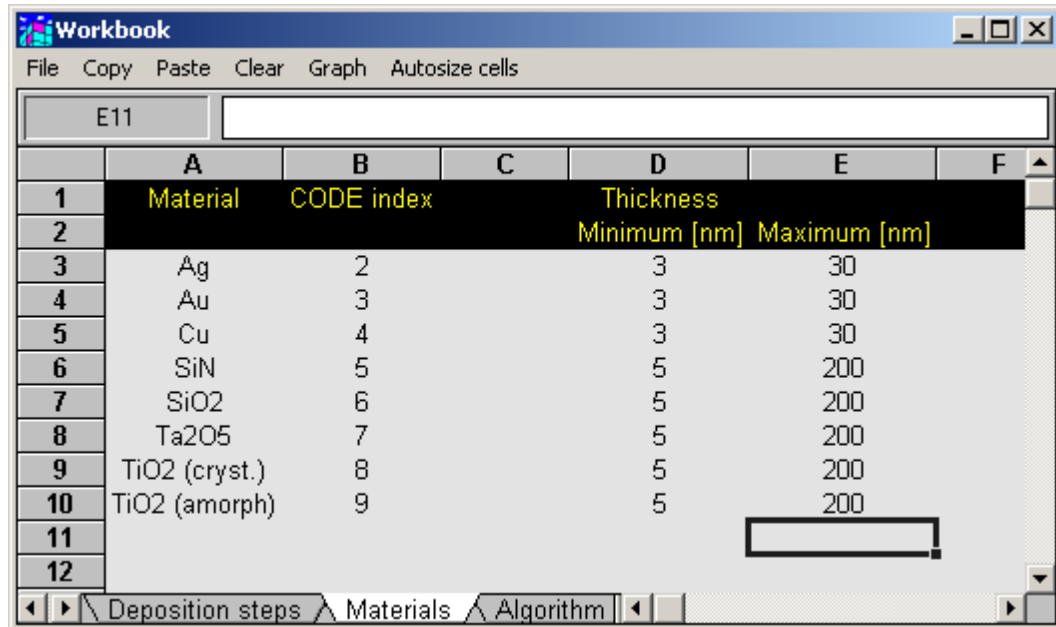


GenetiCode consists of the main window and two sub-objects: A **workbook with user-defined definitions** and the underlying **CODE program** that contains the optical model and does all spectral computations.

The buttons to the left are used to access the sub-objects and to control the program flow. Information on the progress of the optimization is given in the upper right corner of the window. The graph in the lower right corner shows the currently selected view of the underlying CODE configuration. In this case it displays the transmittance spectrum of the air-silicon interface.

2.2 Step 1: Definition of the available materials

First we have to tell *GenetiCode* which materials can be deposited with our equipment. Press the **Definitions** button. The following window opens showing a workbook with several worksheets:

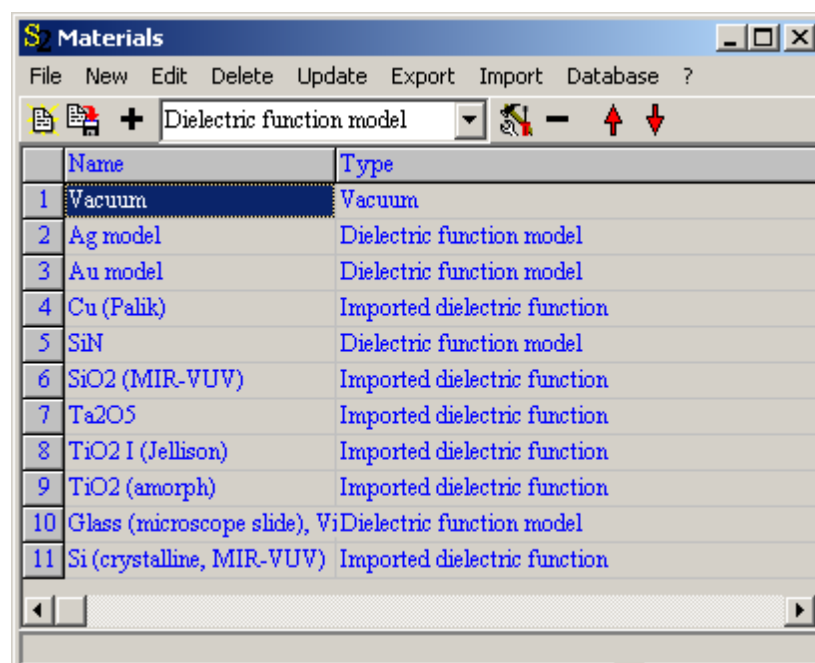


	A	B	C	D	E	F
1	Material	CODE index	Thickness			
2			Minimum [nm]	Maximum [nm]		
3	Ag	2	3	30		
4	Au	3	3	30		
5	Cu	4	3	30		
6	SiN	5	5	200		
7	SiO2	6	5	200		
8	Ta2O5	7	5	200		
9	TiO2 (cryst.)	8	5	200		
10	TiO2 (amorph)	9	5	200		
11						
12						

At the bottom, the 'Materials' worksheet is selected.

If not yet visible, select the worksheet 'Materials' as indicated. There are 4 columns to be filled. The first one called 'Material' holds the names of the materials that can be produced with your deposition devices. You can freely set names here. However, the corresponding optical constants must occur in the list of materials in the underlying CODE configuration. The connection to the CODE list is made by the column called 'CODE index'. CODE index 2 means in this case that the optical constants for the material called 'Ag' are to be taken from the second item in the material list of CODE.

In order to lookup index values it is useful to inspect the material list of CODE. Go back to the *GenetiCode* main window and press the 'Open CODE' button. This opens CODE. Use the **Objects | Materials** menu command to display the list of materials:

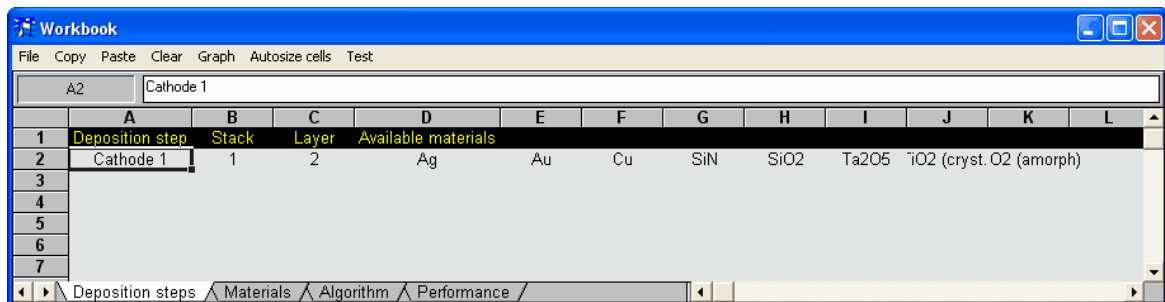


	Name	Type
1	Vacuum	Vacuum
2	Ag model	Dielectric function model
3	Au model	Dielectric function model
4	Cu (Palik)	Imported dielectric function
5	SiN	Dielectric function model
6	SiO2 (MIR-VUV)	Imported dielectric function
7	Ta2O5	Imported dielectric function
8	TiO2 I (Jellison)	Imported dielectric function
9	TiO2 (amorph)	Imported dielectric function
10	Glass (microscope slide), Vi	Dielectric function model
11	Si (crystalline, MIR-VUV)	Imported dielectric function

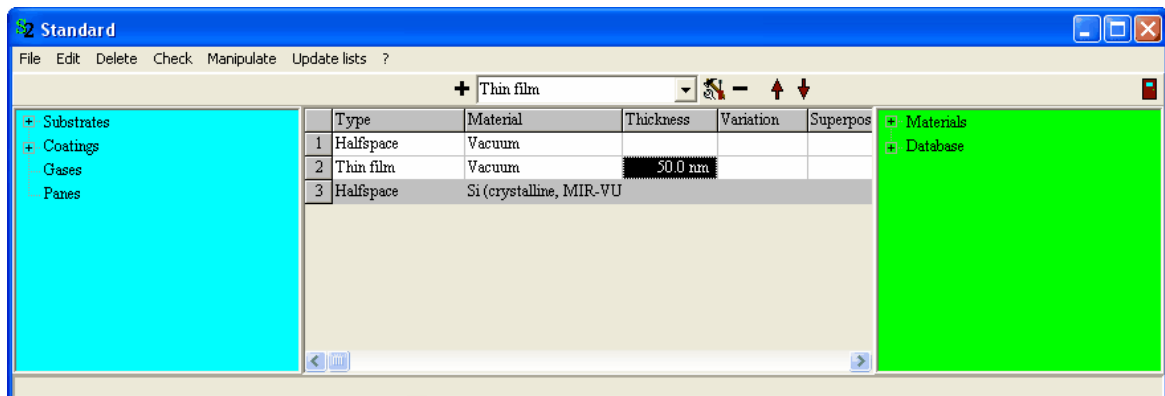
All the used optical constants have been taken from the CODE database. Note that the names of the materials in the database and in *GenetiCode* may be different. Doing your own design work, please check very carefully the material assignments and the correct CODE index values. For each material you have to specify the minimum and maximum thickness values you can produce. All thickness values must be given in nanometers.

2.3 Step 2: Deposition steps

Now we have to define the available deposition steps. Open the workbook sheet 'Deposition steps':



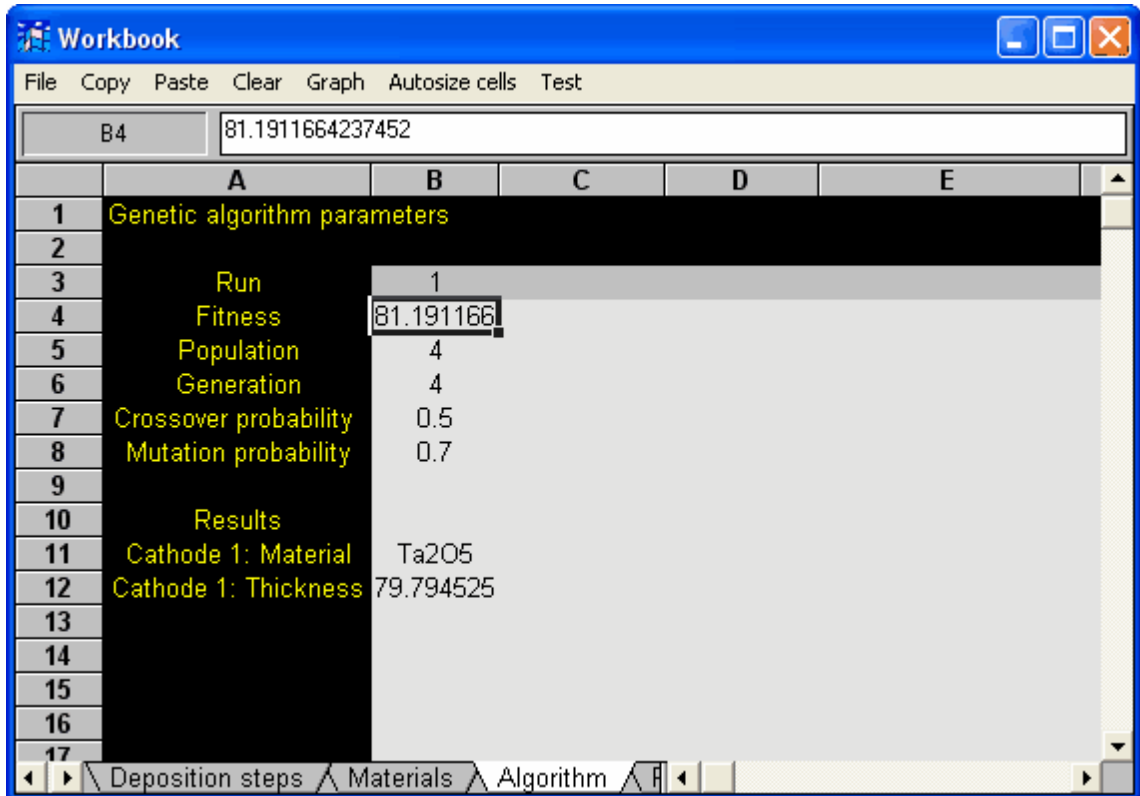
The column 'Deposition step' holds the names of the individual deposition devices. The connection between the deposition device and the optical model is made by the columns 'Stack' and 'Layer'. They represent the number of the layer stack in CODE (in almost all cases this will be 1 because you usually use only one layer stack) and the number of the layer within that layer stack. In order to do the correct assignments you should open the layer stack in CODE (**Objects|Layer stacks**):



Here we use only layer number 2 (row 2, right now filled with 'Vacuum', thickness: 50 nm). The workbook section 'Available materials' starting at cell D2 lists the materials that are available for this layer. To list up all materials *GenetiCode* scans to the right until the first empty cell is found. The names used in the section 'Available materials' must exactly match those defined on the worksheet 'Materials'. To be safe, use copy&paste to prepare the list for each layer. Later on we will use more than just one layer for the anti-reflection coating.

2.4 Step 3: Algorithm parameters

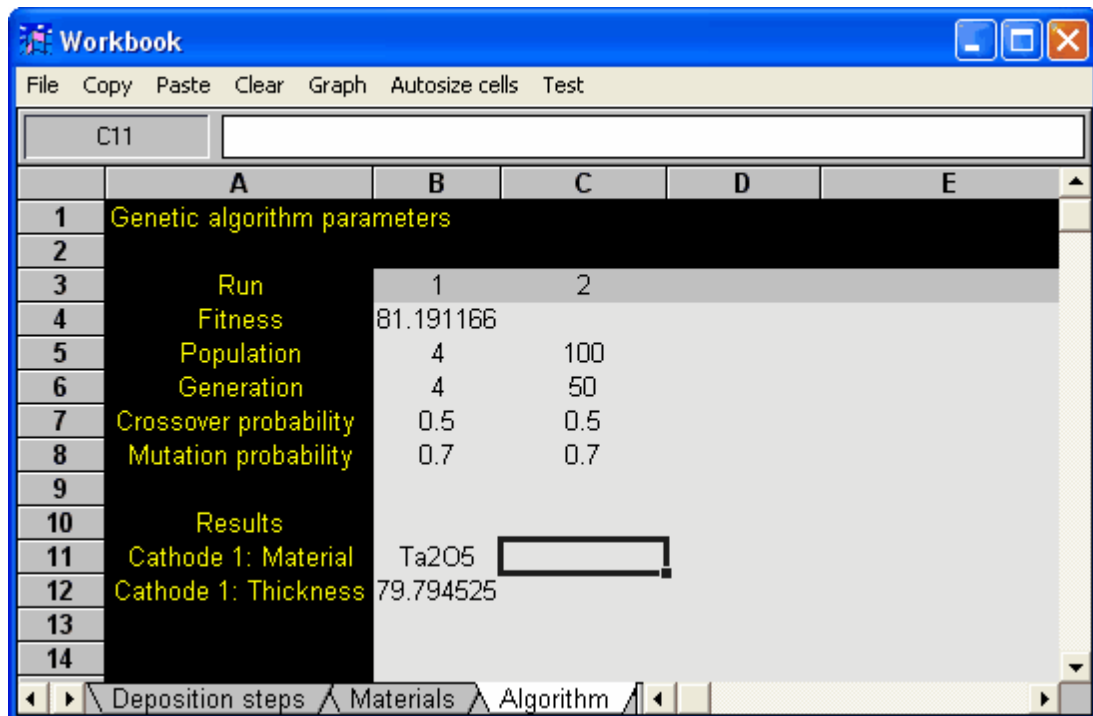
Before we start the automatic design the algorithm needs some control parameters. Open the workbook sheet 'Algorithm':



Here you can define the parameters for several evolution runs, each one being described by a column. Start at column B with the first run. Row 'Run' just holds a name for the run (usually a counting number, but it can also be a text phrase). The 'Fitness' row will display the highest fitness achieved after the evolution. Under 'Population' you can set how many individual coatings are used for evolution. 'Generations' sets the maximum number of generations. *GenetiCode* will stop after this number has been reached. The rows 'Crossover probability' and 'Mutation probability' hold the crossover and mutation probabilities, respectively.

The 'Results' section stores the 'genes' of the best individual after the evolution. These values are used to reconstruct the layer stack if you want to inspect the result of this run. Do not modify these values and do not try to understand their meaning.

In this first example we will just do one very short run with a population of 4 and 4 generations as indicated and a second (longer) run with a population of 100 and 50 generations. The worksheet 'Algorithm' should then look like this:



2.5 Step 4: Automatic design

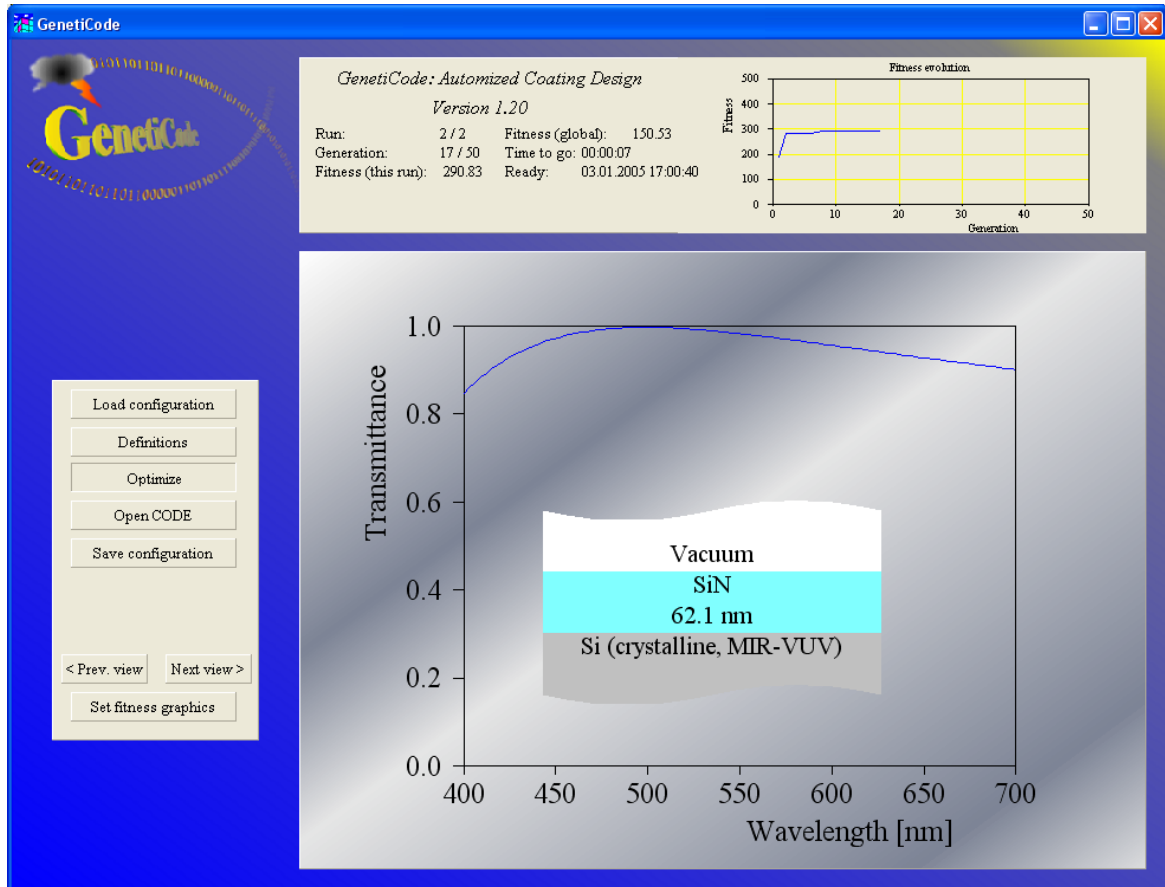
Start the evolution

Now we are ready to start the automatic design. Go back to the main window and press the 'Optimize' button.

Now some activity starts and the upper right corner of the main window displays some information. 'Run' shows the number of the current run and the total number of runs. 'Generations' the current generation and the total number of generations to be processed. The highest fitness of the current run and in the case of more than one run the overall highest fitness are given as well.

Based on the computational time needed for the work already done, *GenetiCode* tries to predict how long it will need for the remaining calculations. It will display the time to go and the data and time of the expected end.

The graphical display is updated after each generation and represents the best solution of the current run:

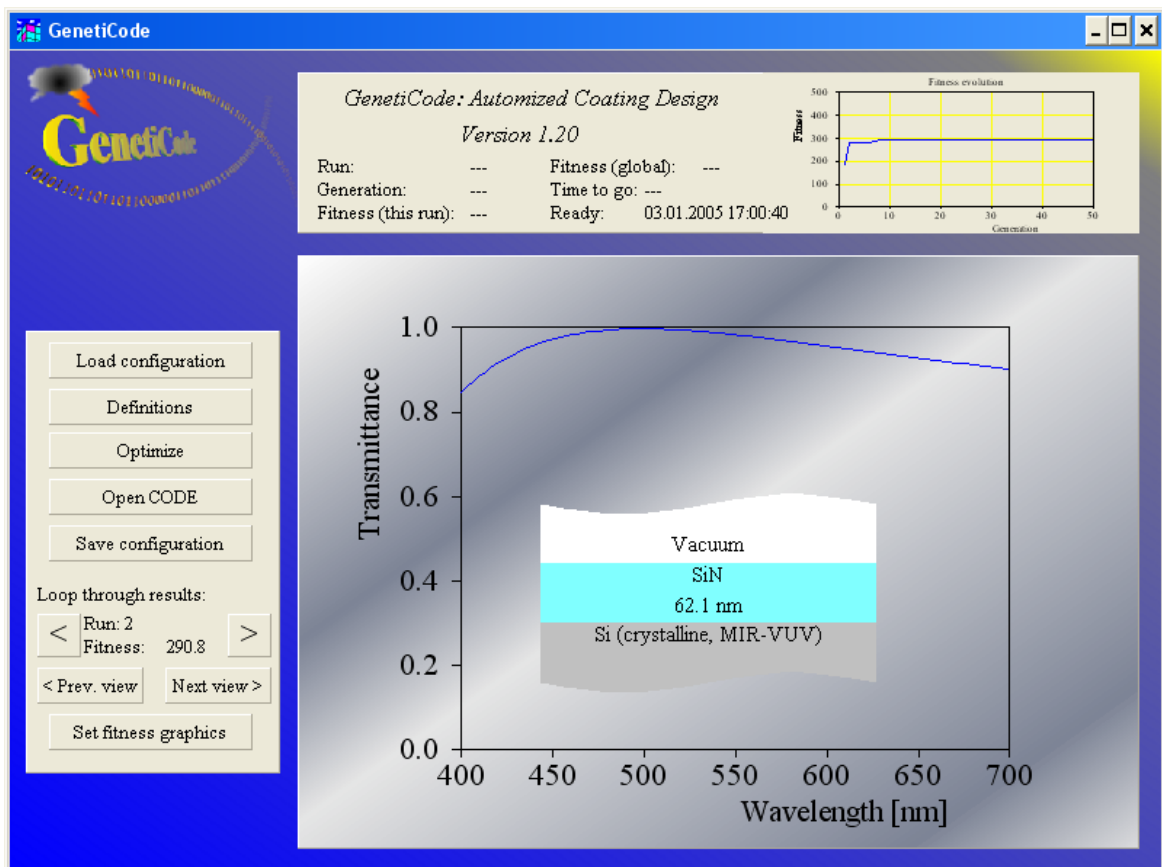
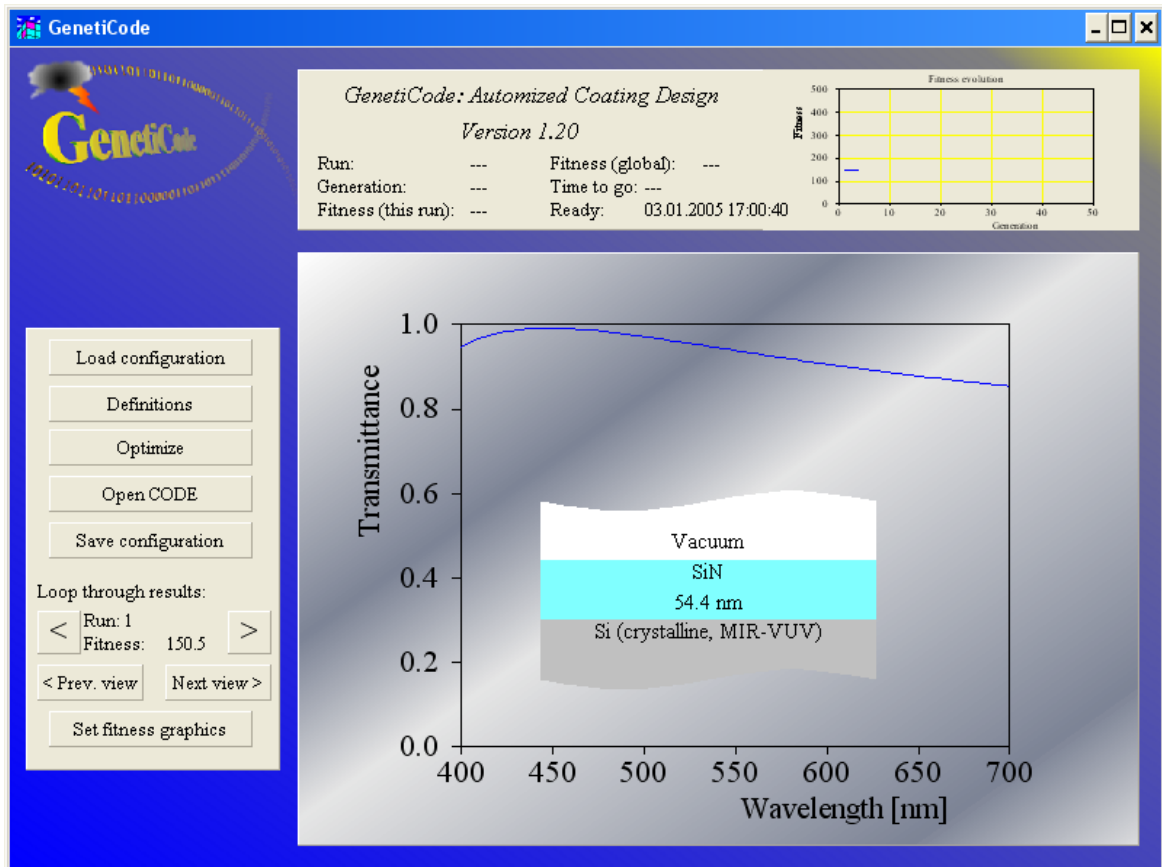


Automatic and manual stop

When all defined runs are done *GenetiCode* will stop automatically. During the numerical evolution work, the 'Optimize' button stays in its down position. Any time you can press it again and tell *GenetiCode* to stop. The program will do some cleaning up steps and then finish with the best solution obtained in the last run.

2.6 Step 5: Inspection of the results

In order to inspect the results of the individual runs you can use the buttons labeled '<' and '>' on the left side of the main window. *GenetiCode* reconstructs the CODE configuration for the best result of this run and updates its view in the main window. The fitness evolution of this run is also restored from the workbook:



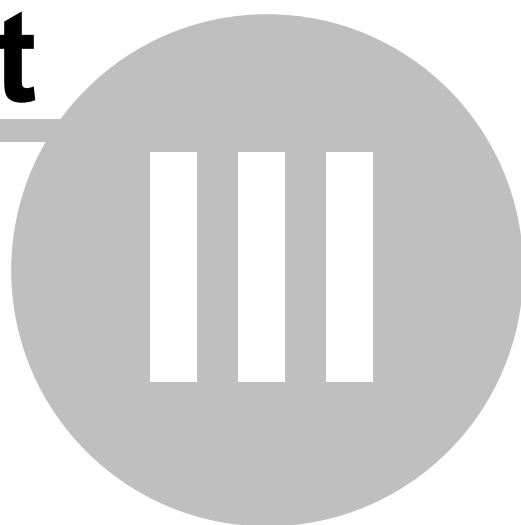
Obviously it is advantageous to display all relevant quantities in the CODE view. If you like, you can define several views in your CODE configuration showing spectra, integral data like color coordinates or whatever you want to see as a result. [GenetiCode](#) lets you switch from view to view with the buttons labeled '< Prev. view' and 'Next view >'.

In order to get all details of the best solution you can open CODE and copy whatever you want to copy (e.g. the layer stack definition).

In case of a successful run you should save the [GenetiCode](#) configuration using the 'Save configuration' button.

More advanced problems are discussed below.

Part



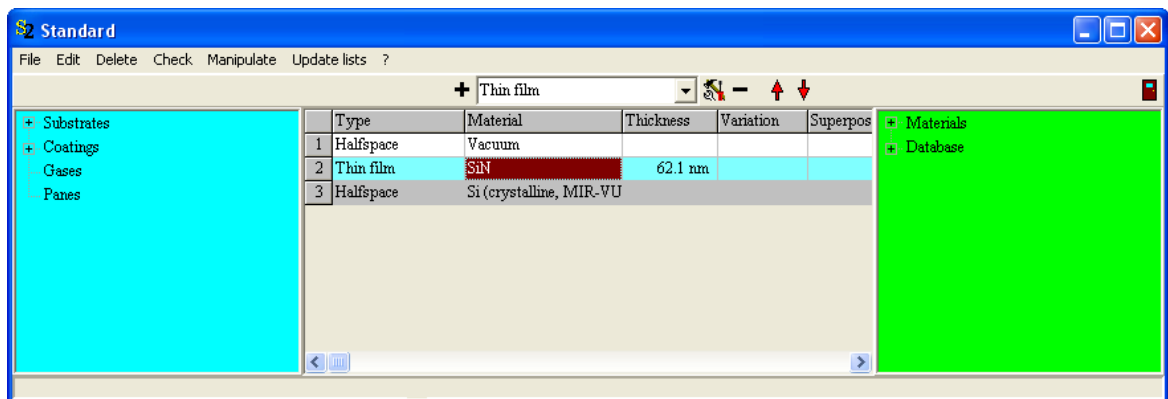
3 A three-layer anti-reflection coating

3.1 Modifications of the first example

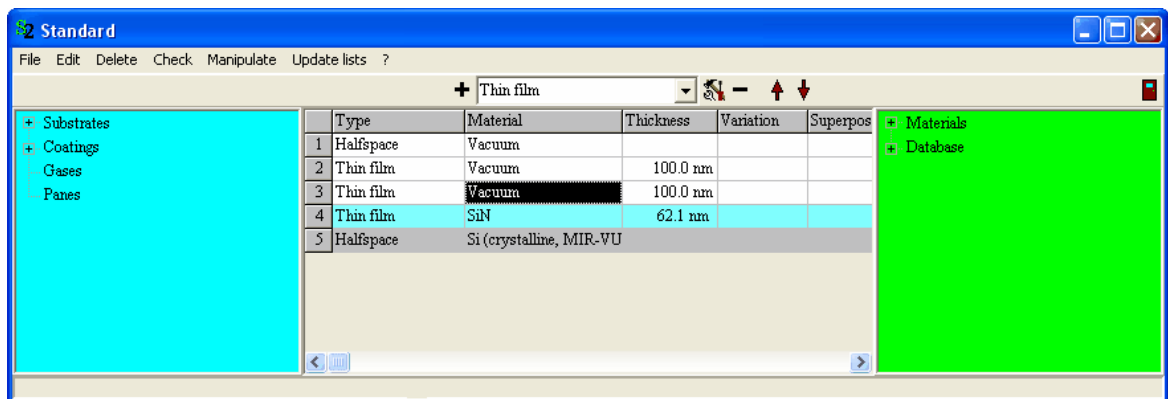
We will now modify the first simple example and let the program design a more advanced three layer anti-reflection coating. This section shows the required steps in detail. If you have closed the program after the first example start *GenetiCode* again. The configuration AR_1layer.gcd contains the result of the first example and will be modified as follows.

Modification of the CODE settings

Use the **Open CODE** command to access CODE and go to the layer stack definition:



Add two thin films above the Si halfspace:



We are not introducing new optical constants in this example. The layer stack modification is the only modification of the CODE configuration.

Changes of the workbook settings

We are going to work with the same collection of possible materials in this example. No new materials need to be defined. Modifications must be done on the sheet 'Deposition steps', of course. Select the description of the first deposition step in row 3 as follows:

	A	B	C	D	E	F	G	H	I	J	K
1	Deposition step	Stack	Layer	Available materials							
2	Cathode 1	1	2	Ag	Au	Cu	SiN	SiO2	Ta2O5	TiO2 (cryst. O2 (amorph))	
3											
4											
5											
6											
7											

Now use the **Copy** command to copy the selection to the clipboard. Place the cursor in the cell A3 and **Paste** the content. Do the **Paste** action again starting at cell A4. The new settings are this:

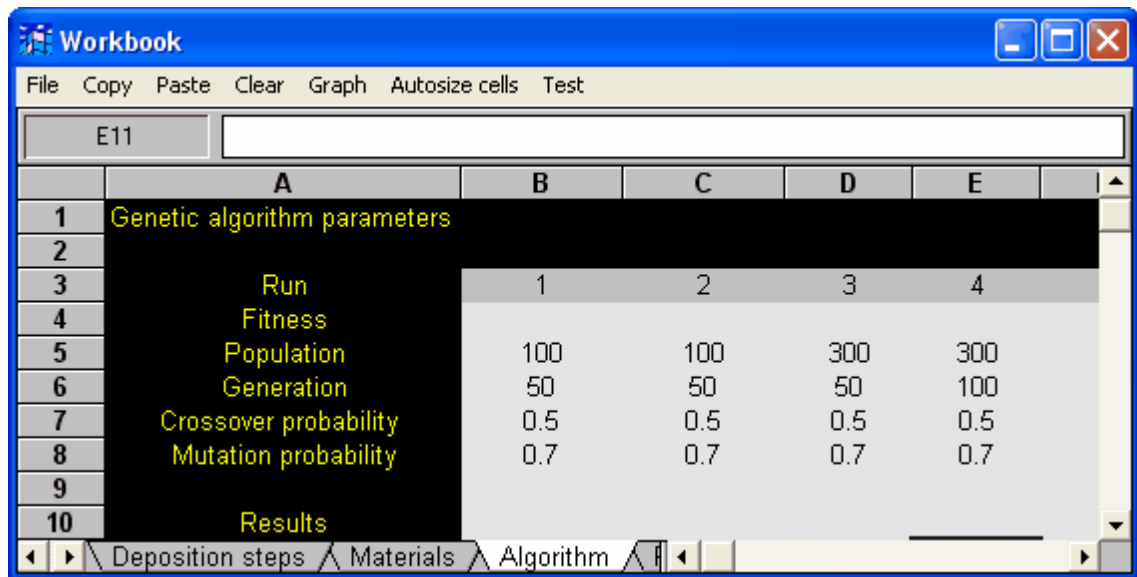
	A	B	C	D	E	F	G	H	I	J	K
1	Deposition step	Stack	Layer	Available materials							
2	Cathode 1	1	2	Ag	Au	Cu	SiN	SiO2	Ta2O5	TiO2 (cryst. O2 (amorph))	
3	Cathode 1	1	2	Ag	Au	Cu	SiN	SiO2	Ta2O5	TiO2 (cryst. O2 (amorph))	
4	Cathode 1	1	2	Ag	Au	Cu	SiN	SiO2	Ta2O5	TiO2 (cryst. O2 (amorph))	
5											
6											
7											

(Alternatively, you could have copied the selection by dragging down the little black rectangle at the lower right corner of the workbook selection)

Change the names of the new deposition steps from 'Cathode 1' to 'Cathode 2' and 'Cathode 3', respectively. Most important, set the values of the layer index in column C to 3 and 4, respectively:

	A	B	C	D	E	F	G	H	I	J	K
1	Deposition step	Stack	Layer	Available materials							
2	Cathode 1	1	2	Ag	Au	Cu	SiN	SiO2	Ta2O5	TiO2 (cryst. O2 (amorph))	
3	Cathode 2	1	3	Ag	Au	Cu	SiN	SiO2	Ta2O5	TiO2 (cryst. O2 (amorph))	
4	Cathode 3	1	4	Ag	Au	Cu	SiN	SiO2	Ta2O5	TiO2 (cryst. O2 (amorph))	
5											
6											
7											

In this more complex design task it is useful to have several runs with larger populations and generations. Change the 'Algorithm' page to the following:



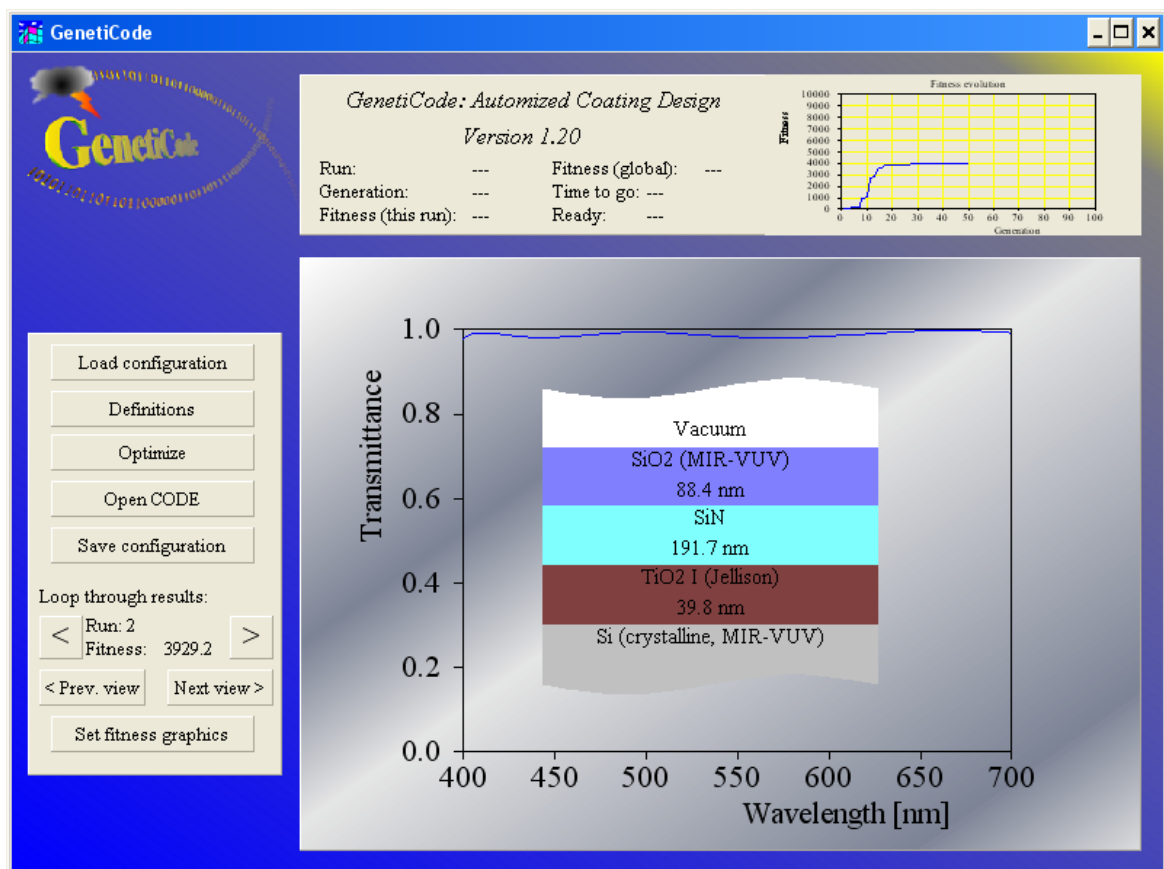
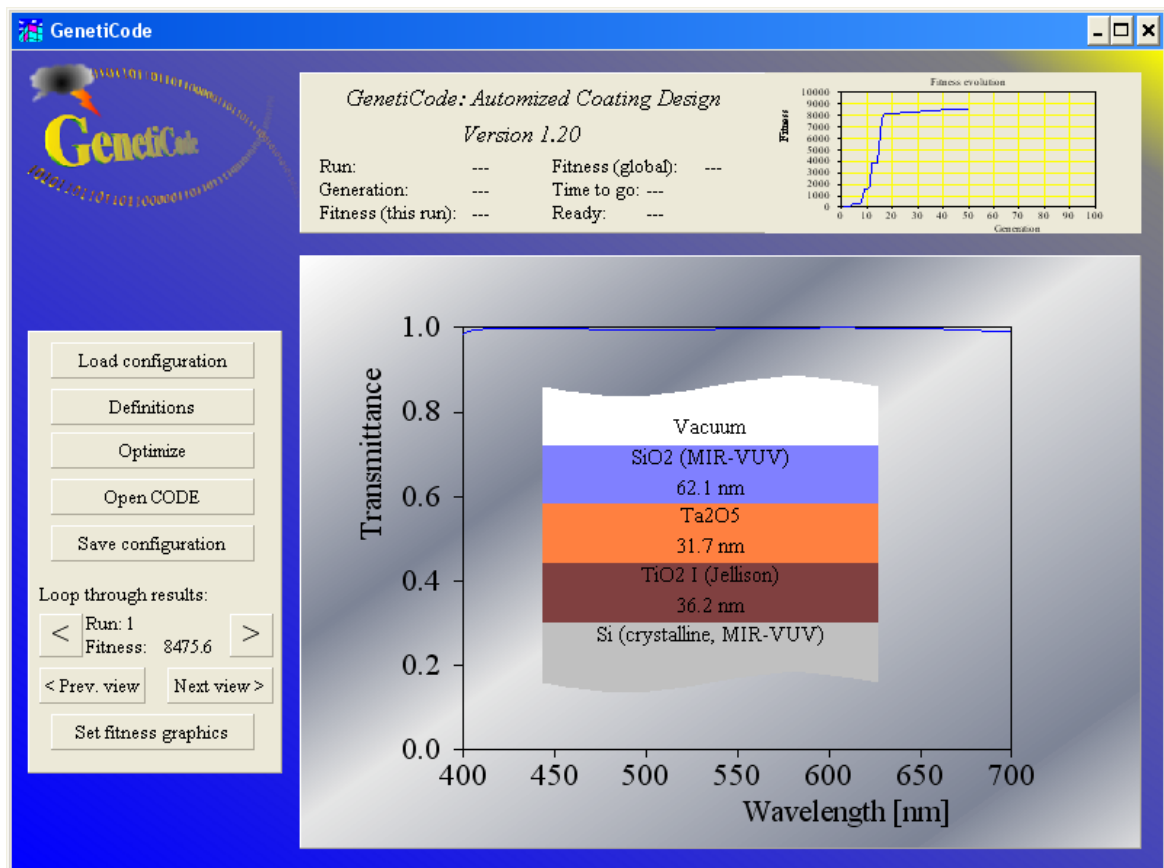
	A	B	C	D	E
1	Genetic algorithm parameters				
2					
3	Run	1	2	3	4
4	Fitness				
5	Population	100	100	300	300
6	Generation	50	50	50	100
7	Crossover probability	0.5	0.5	0.5	0.5
8	Mutation probability	0.7	0.7	0.7	0.7
9	Results				
10					

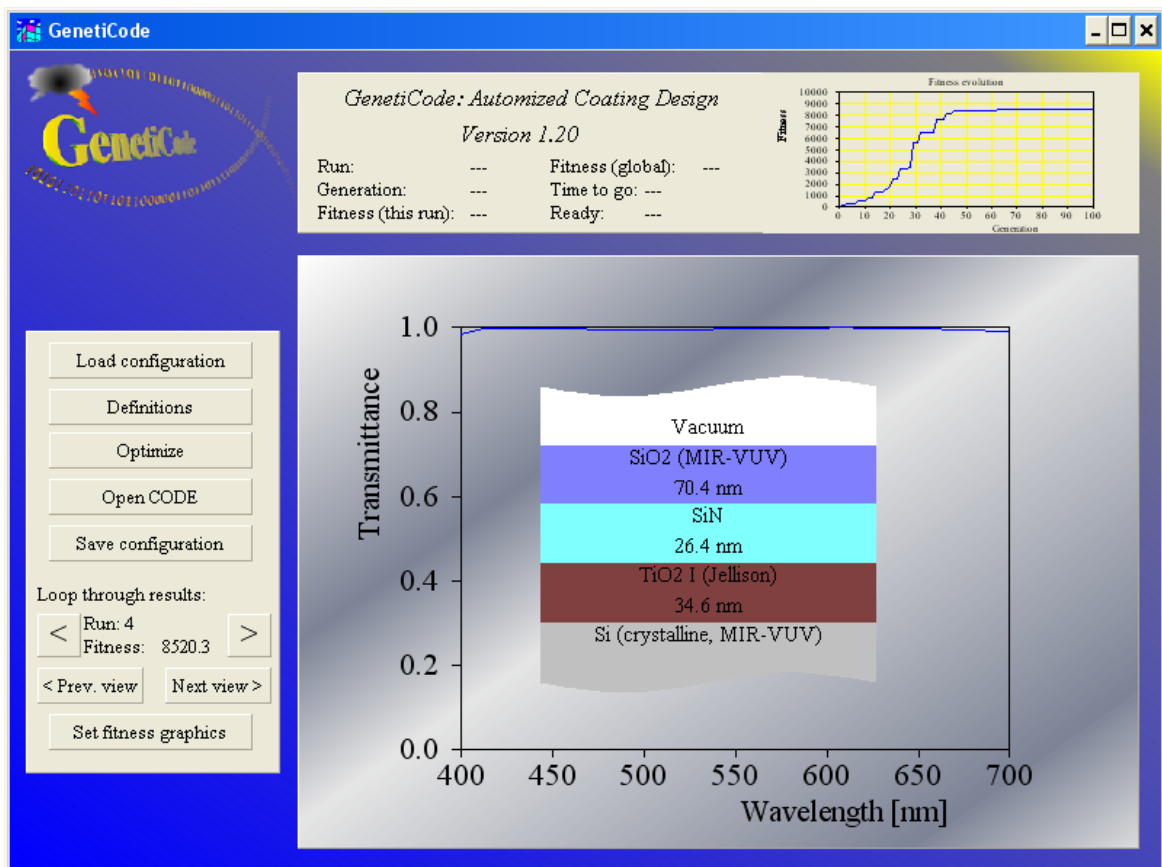
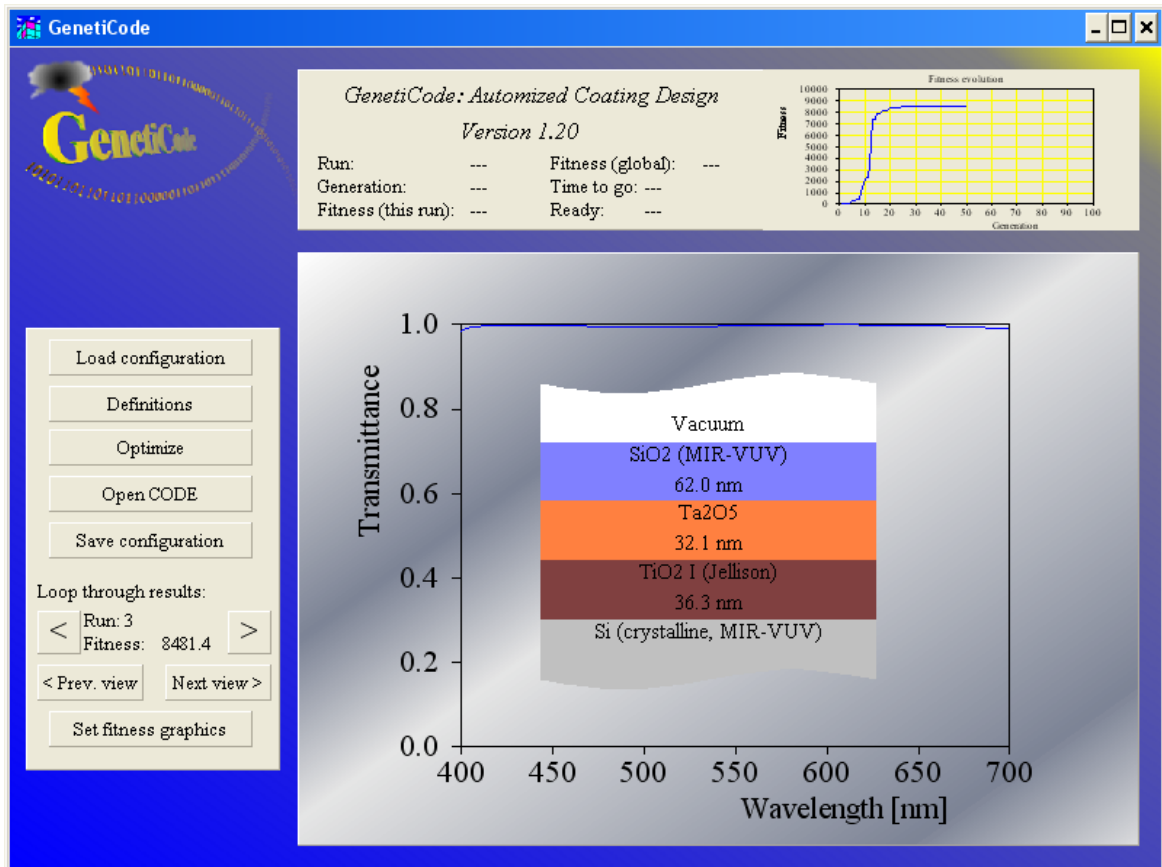
This is all we have to change.

Press the **Optimize** button and watch the evolution of the system.

3.2 Results

In this case the program takes a little longer and the individual runs show real evolutions, i.e. a noticeable development of the fitness from generation to generation. My results are stored in the configuration AR_Si_3layers.gcd which is distributed with the [GenetiCode](#) software. I have got the following solutions:





Note that the best solutions (Run 3 and Run 4) have found different material selections for the layer stack. The fitness is almost the same in Run 1, 3 and 4 whereas Run 2 is much worse. This shows that you should not rely on a single run in order to solve a design problem.

There is no proof that Run 4 represents the best solution. In order to see if there are different and even better solutions you have to re-run the evolution, eventually with different settings for the parameters of the algorithm.

If you want to keep a configuration you can press the 'Save configuration' button and store the present status to a file (that you can re-load using the 'Load configuration' button). The present configuration is contained in the file AR_Si_3layers.gcd which is distributed with [GenetiCode](#).

Part

IV

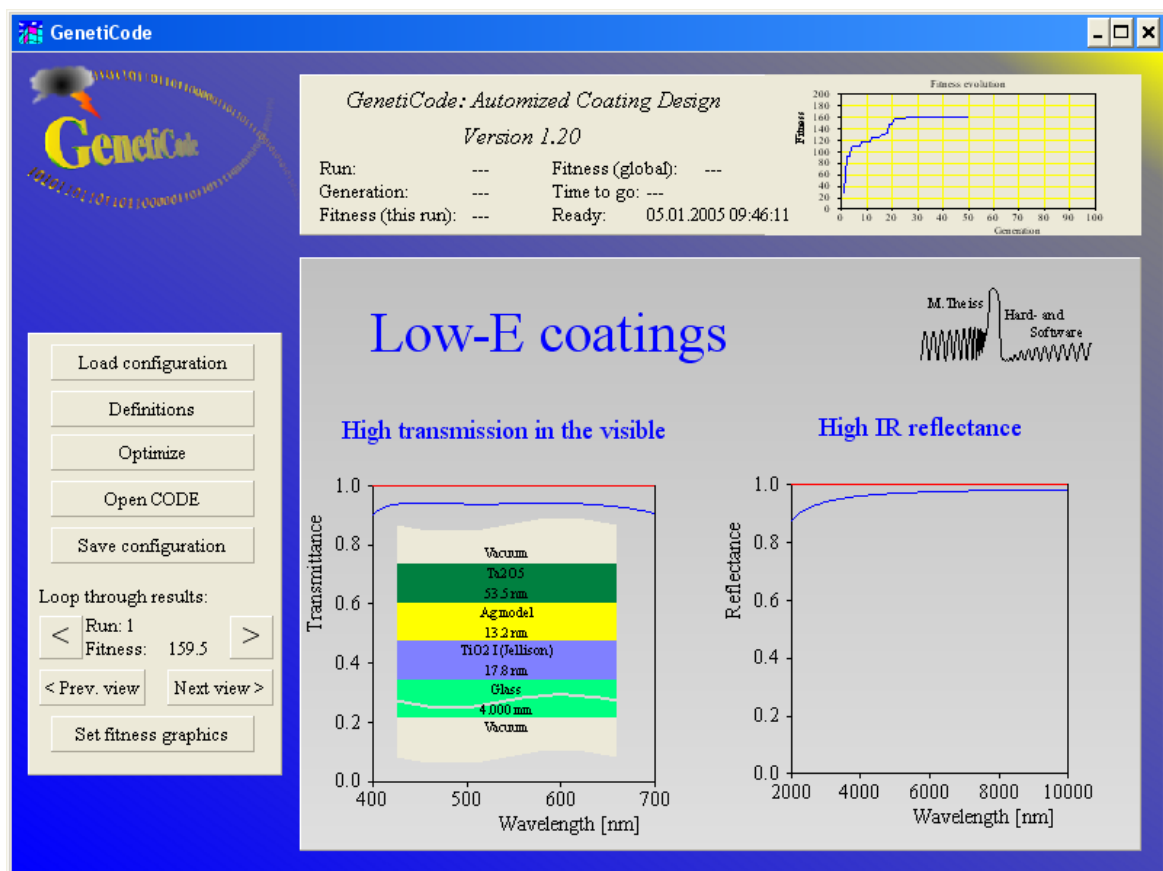
4 'Invention' of low-E coatings

4.1 Three layer coating

This example shows the 'invention' of the well-known basic layer stack for simple low-E coatings. The invention is achieved completely automatic - you specify the wanted optical properties and [GenetiCode](#) finds the solution.

The goal of low-E coatings is to reduce the infrared emission of glass panes while maintaining the transparency in the visible. This way the transfer of energy from the warm interior pane to the cold exterior pane of a double glazing by infrared radiation is reduced. Let's now try if [GenetiCode](#) can find a good solution for this problem.

Using the 'Load configuration' button load the configuration low_e_3layers.gcd:



This configuration shows the problem of an uncoated pane: Whereas the transmittance in the visible is high the reflectance in the infrared is very low. Since also the IR transmittance is zero (not shown here) glass is a good absorber for infrared radiation. A good absorber is also a good emitter - which is going to be avoided by a suitable coating. The red lines show the target spectra: 100% transmittance in the visible and 100% reflectance in the IR.

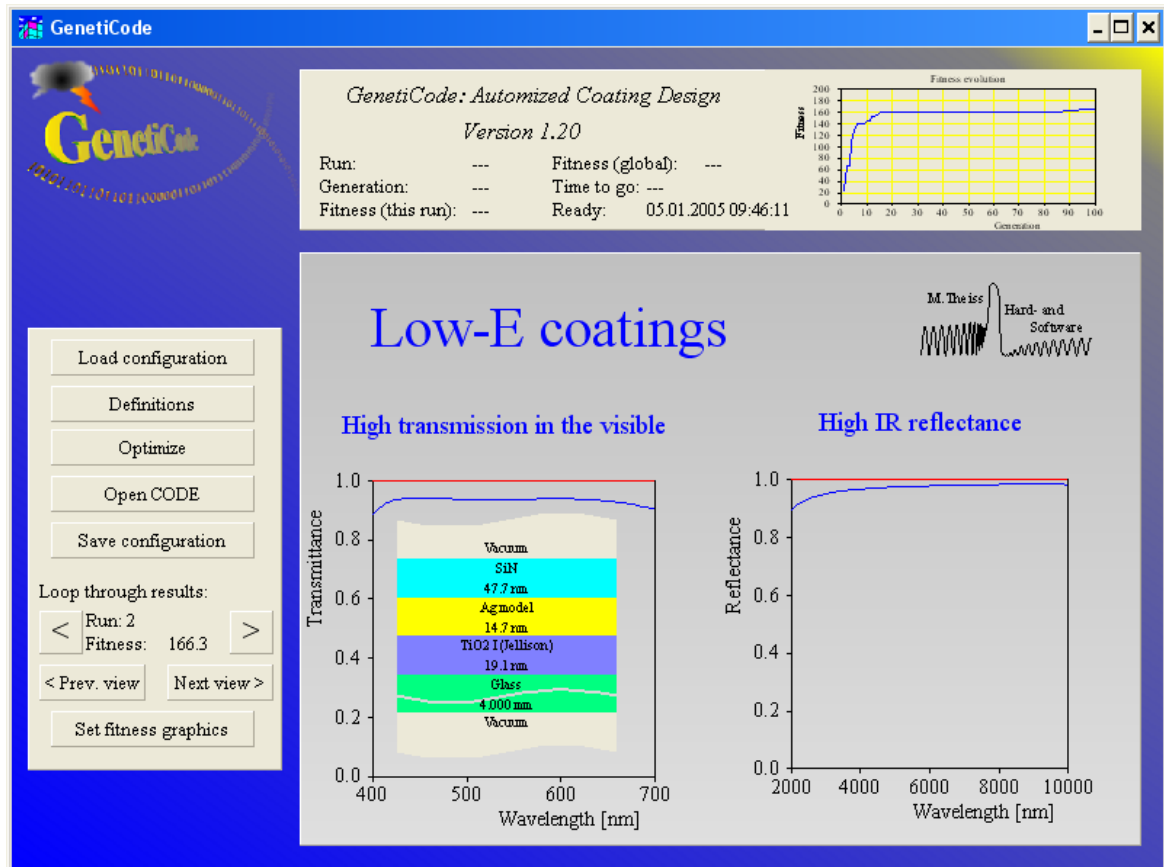
Three deposition steps are used in this first low-E example. The available materials are the following:

	A	B	C	D	E	F
1	Material	CODE index	Thickness			
2			Minimum [nm]	Maximum [nm]		
3	Ag	2	3	30		
4	Au	3	3	30		
5	Cu	4	3	30		
6	SiN	5	5	100		
7	SiO2	6	5	100		
8	Ta2O5	7	5	100		
9	TiO2 (cryst.)	8	5	30		
10	TiO2 (amorph)	9	5	30		
11						
12						

All materials may be used in each deposition step - let *GenetiCode* find out what is the right combination. We do a short test with 2 runs:

	A	B	C
1	Genetic algorithm parameters		
2		1	2
3	Run	1	2
4	Fitness	159.4671677	166.2658516
5	Population	200	100
6	Generations	50	100
7	Crossover probability	0.8	0.8
8	Mutation probability	0.8	0.8
9			
10			

Running the optimization you can watch how the quality of the coating increases. In my case in only a few seconds a quite good solution has been found which is then slowly improved. The best solution in run 2 is this:



This is a typical basic low-E coating which has been invented several years ago by a lot of human thinking. With *GenetiCode* you could have 'invented' it by just stating the problem and pressing the 'Optimize' button.

4.2 Five layer coating

In most cases a design can be improved by adding more layers. Here we try to improve the 3 layer low-E coating found before by adding two additional layers, i.e. working with a 5 layer system. Again no restrictions on the material selection for each deposition step is made. The configuration `low_e_5layers.gcd` contains this approach.

Several runs have been performed with the following parameters and results:

Workbook

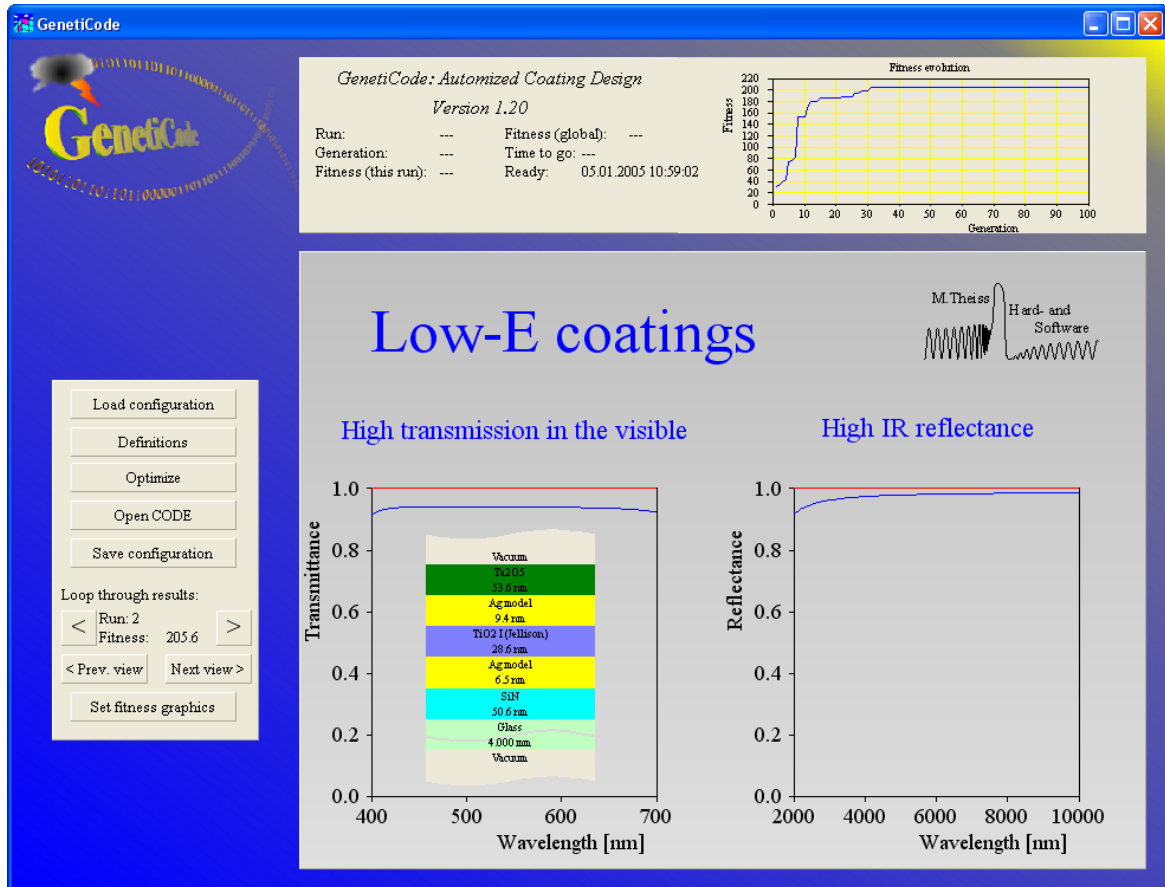
File Copy Paste Clear Graph Autosize cells Test

C19	Ta2O5					
	A	B	C	D	E	F
1	Genetic algorithm parameters					
2						
3	Run Fitness Population Generations Crossover probability Mutation probability	1	2	3	4	5
4		203.0705422	205.6389625	161.9700344	173.0814279	177.4227611
5		100	100	100	100	100
6		100	100	100	100	100
7		0.8	0.8	0.8	0.8	0.8
8		0.8	0.8	0.8	0.8	0.8
9						
10						
11	Cathode 1: Material	SiN	SiN	SiN	SiO2	SiO2
12	Cathode 1: Thickness	40.01787567	50.56136322	10.27818871	99.91457367	75.56376648
13	Cathode 2: Material	Ag	Ag	SiN	SiN	SiO2
14	Cathode 2: Thickness	7.043913841	6.490401268	5.441496372	23.39196205	91.08971405
15	Cathode 3: Material	SiN	TiO2 (cryst.)	TiO2 (cryst.)	TiO2 (cryst.)	TiO2 (cryst.)
16	Cathode 3: Thickness	70.83963013	28.59380913	14.25583172	12.99616241	19.22151375
17	Cathode 4: Material	Ag	Ag	Ag	Ag	Ag
18	Cathode 4: Thickness	6.893856525	9.378756523	13.03717422	14.24718857	14.52910042
19	Cathode 5: Material	SiO2	Ta2O5	Ta2O5	SiN	SiN
20	Cathode 5: Thickness	66.17508698	53.60826874	53.19399261	45.96063232	46.88527679
21						
22						

Deposition steps Materials Algorithm Performance

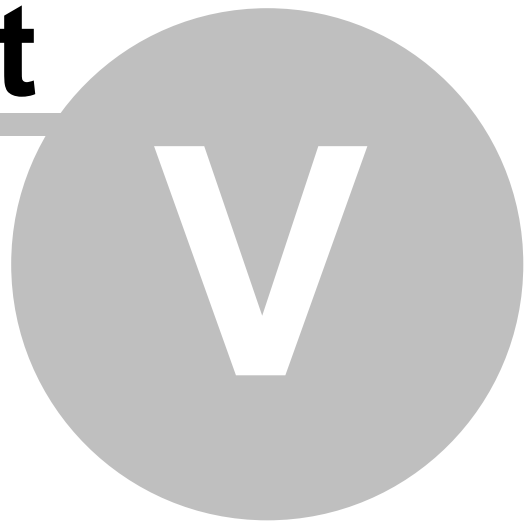
With the exception of run 3 the achieved fitness values are all above 166 which was the best result for the 3 layer approach.

The improved result with respect to the best 3 layer solution has been achieved by the introduction of a second silver layer:



Note that double silver layers are used in actual low-E and solar control products. Within a few minutes (on a 2 GHz PC) this new design was (completely automatically) achieved by [GenetiCode](#).

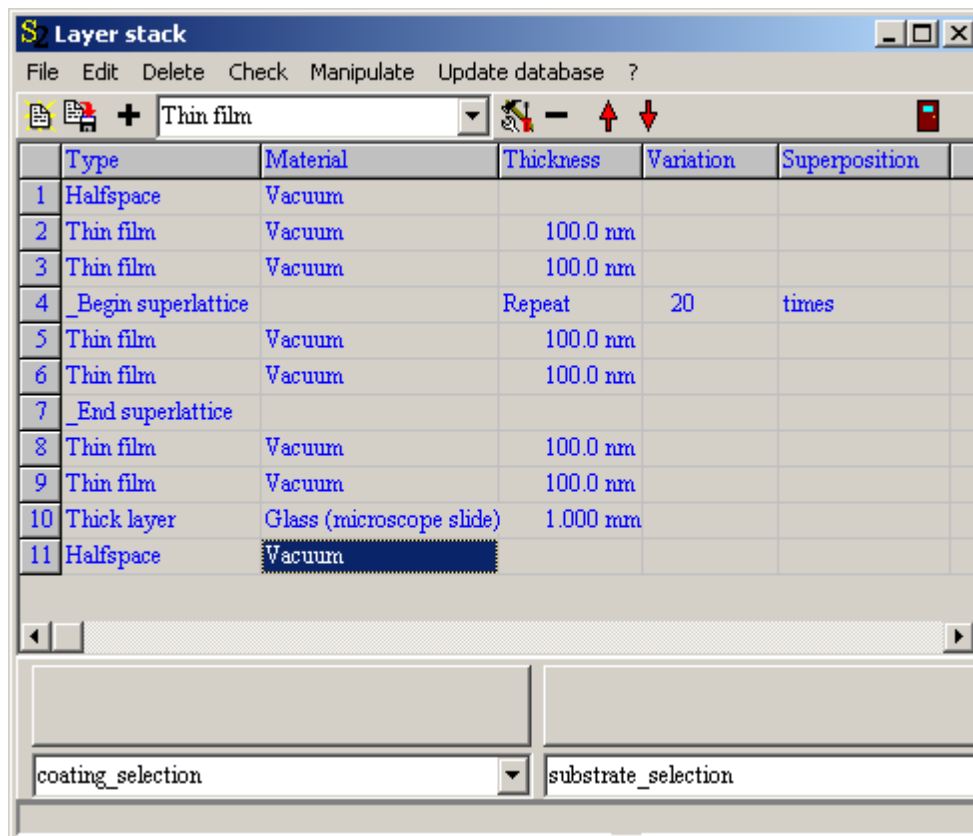
Part



5 Optical filters

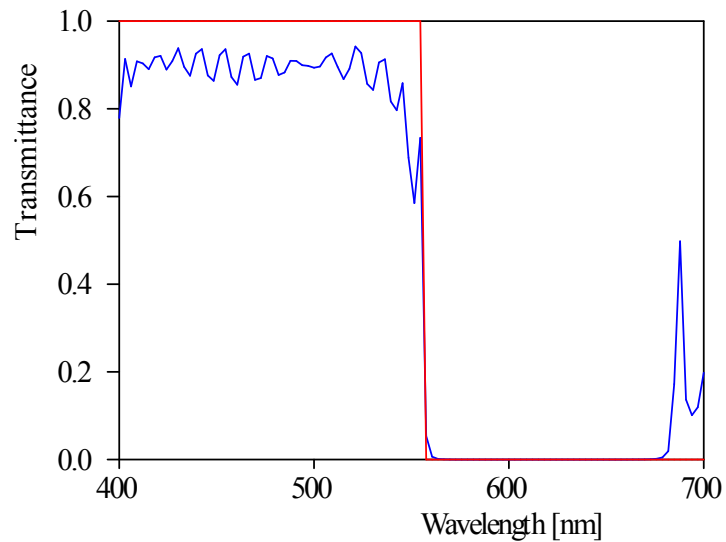
5.1 Edge filters

The automatic design of an edge filter is shown in this section. The layer stack involves a superlattice which will serve as an optical Bragg reflector. Its high reflectivity (close to 1) will be used to suppress the transmission in a broad spectral range. Around the superlattice there are some additional thin films which might be useful for the optimization:



However, we actually do not need to understand the function of the individual layers as long as we know what kind of ingredients could be useful.

The target spectrum for the design is a sharp edge (the red spectrum in the following, computed with the Data factory tool using a user-defined formula):



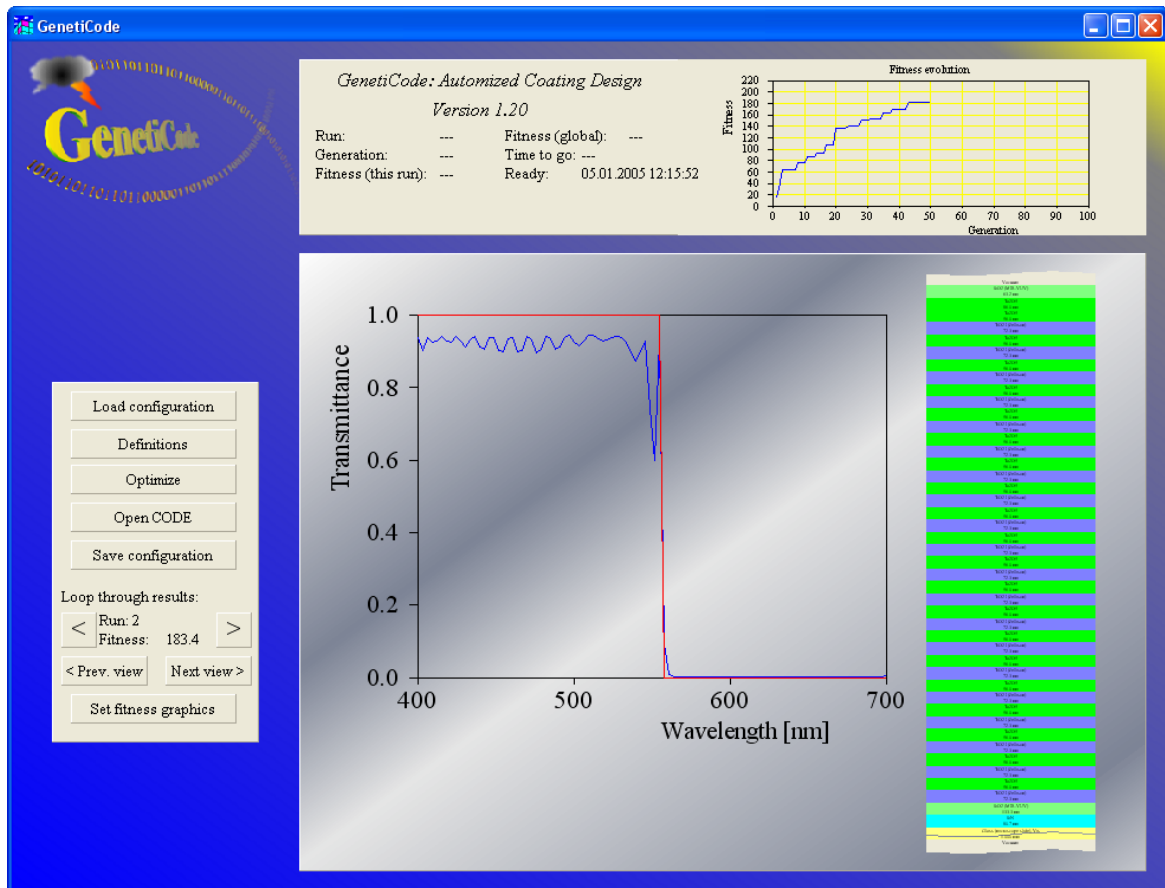
For the 6 layers only oxides or nitrides are allowed. The assignments are as follows:

Workbook								
File Copy Paste Clear Graph Autosize cells								
A2		1						
	A	B	C	D	E	F	G	H
1	Deposition step	Stack	Layer	Available materials				
2	1	1	2	SiO2	SiN	Ta2O5	TiO2 (cryst.)	
3	2	1	3	SiO2	SiN	Ta2O5	TiO2 (cryst.)	
4	3	1	5	SiO2	SiN	Ta2O5	TiO2 (cryst.)	
5	4	1	6	SiO2	SiN	Ta2O5	TiO2 (cryst.)	
6	5	1	8	SiO2	SiN	Ta2O5	TiO2 (cryst.)	
7	6	1	9	SiO2	SiN	Ta2O5	TiO2 (cryst.)	
8								
9								

Several runs have been tried this time:

Workbook					
File Copy Paste Clear Graph Autosize cells Test					
F27					
	A	B	C	D	E
1	Genetic algorithm parameters				
2					
3	Run	1	2	3	4
4	Fitness	72.94516973	183.3729525	174.0526265	150.7910459
5	Population	500	1000	1000	1000
6	Generations	20	50	100	100
7	Crossover probability	0.7	0.7	0.7	0.7
8	Mutation probability	0.5	0.8	0.8	0.8
9					
10					

The best result was achieved in run 2:

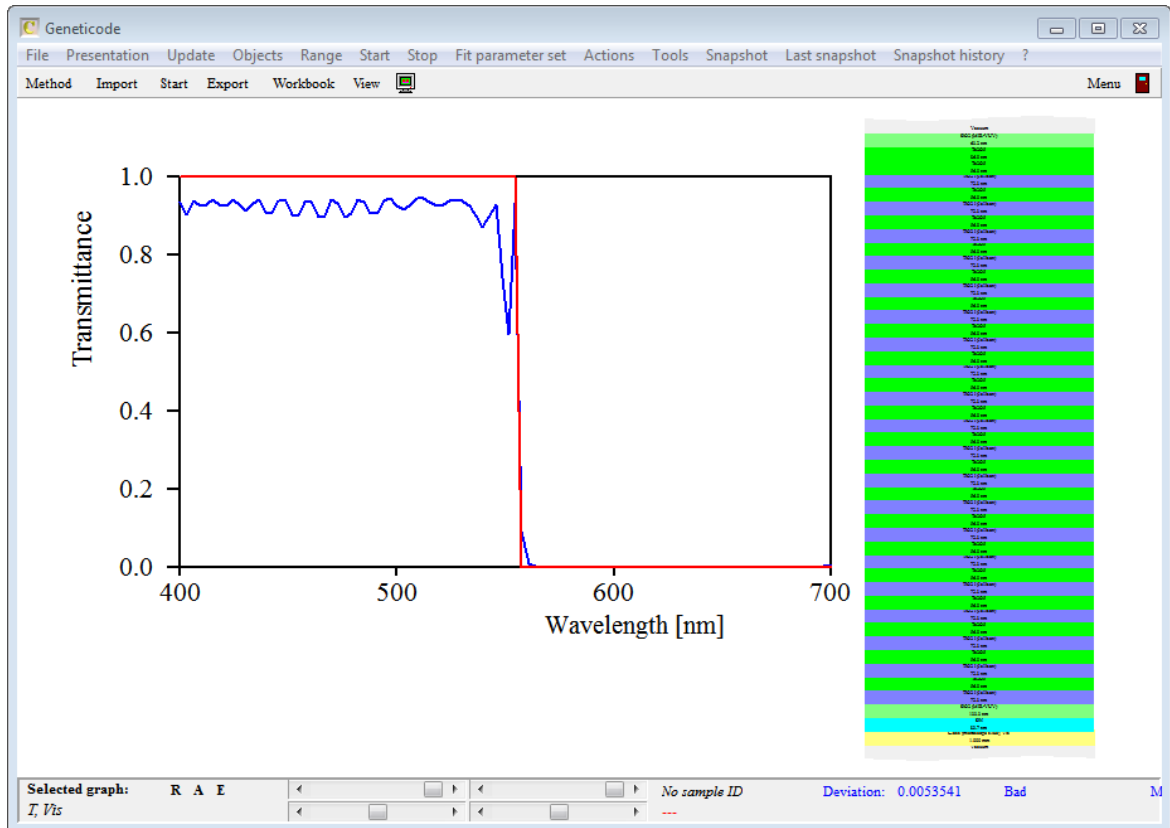


The layer stack design is this:

	Type	Material	Thickness	Variation	Superposition
1	Halfspace	Vacuum			
2	Thin film	SiO ₂ (MIR-VUV)	194.3 nm		
3	Thin film	Ta ₂ O ₅	162.5 nm		
4	_Begin superlattice		Repeat	20	times
5	Thin film	TiO ₂ I (Jellison)	79.8 nm		
6	Thin film	SiO ₂ (MIR-VUV)	57.9 nm		
7	_End superlattice				
8	Thin film	Ta ₂ O ₅	144.2 nm		
9	Thin film	SiO ₂ (MIR-VUV)	76.1 nm		
10	Thick layer	Glass (microscope slide)	1.000 mm		
11	Halfspace	Vacuum			

Note that this result of the evolutionary algorithm can be significantly improved by some manual refinements. In order to make progress we have to start with the existing layer stack, convert the optical superlattice, i.e. the strict 20-fold repetition of the double layer, into 40 single layers, and then optimize the layer thicknesses in CODE using the downhill simplex method. It would not be advantageous to optimize that many layers with the genetic method itself.

Here is how to proceed: Click the 'Open CODE' button to open the CODE instance that works inside GenetiCode:



Press F7 and open the only layer stack in the configuration:

Layer stack				
File Check Edit Manipulate Update lists Fluctuation Delete Delete all ? Wizards				
+ Thin film				
Substrates	Type	Material	Thickness	Variation
Panes	1 Halfspace	Vacuum		
Foils	2 Thin film	SiO2 (MIR-VUV)	63.2 nm	
Stacks in this configuration	3 Thin film	Ta2O5	86.0 nm	
Coatings	4 _Begin superlattice		Repeat	20
New single layers	5 Thin film	Ta2O5	56.0 nm	
	6 Thin film	TiO2 I (Jellison)	72.3 nm	
	7 _End superlattice			
	8 Thin film	SiO2 (MIR-VUV)	133.3 nm	
	9 Thin film	SiN	80.7 nm	
	10 Thick layer	Glass (microscope slide)	1.000 mm	
	11 Halfspace	Vacuum		

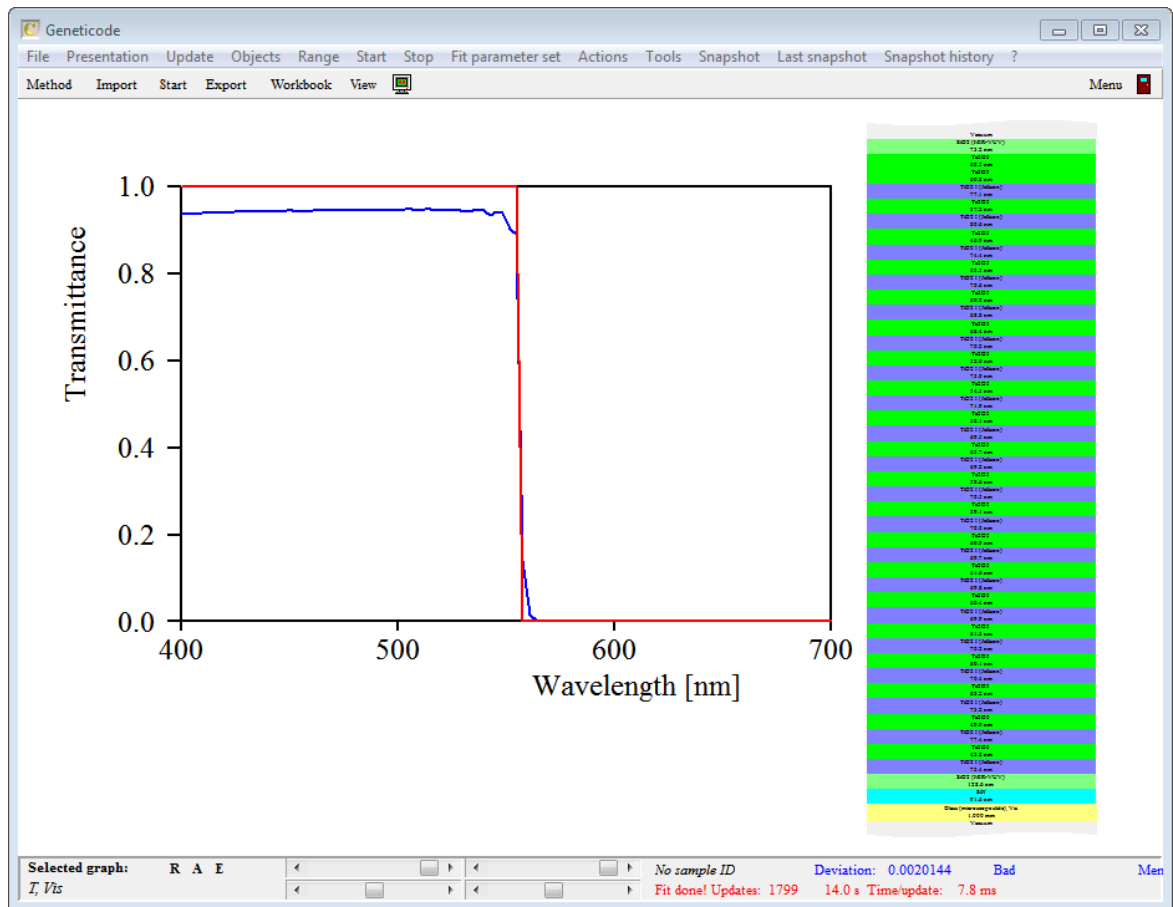
Now execute the local menu command "Manipulate/Convert superlattices into single layers" (which has been introduced with object generation 4.01) and verify that the converted layer stack has many single layers instead of a superlattice structure:

+ Thin film					
	Type	Material	Thickness	Variation	Sup
1	Halfspace	Vacuum			
2	Thin film	SiO ₂ (MIR-VUV)	63.2 nm		
3	Thin film	Ta ₂ O ₅	86.0 nm		
4	Thin film	Ta ₂ O ₅	56.0 nm		
5	Thin film	TiO ₂ I (Jellison)	72.3 nm		
6	Thin film	Ta ₂ O ₅	56.0 nm		
7	Thin film	TiO ₂ I (Jellison)	72.3 nm		
8	Thin film	Ta ₂ O ₅	56.0 nm		
9	Thin film	TiO ₂ I (Jellison)	72.3 nm		
10	Thin film	Ta ₂ O ₅	56.0 nm		
11	Thin film	TiO ₂ I (Jellison)	72.3 nm		
12	Thin film	Ta ₂ O ₅	56.0 nm		
13	Thin film	TiO ₂ I (Jellison)	72.3 nm		
14	Thin film	Ta ₂ O ₅	56.0 nm		
15	Thin film	TiO ₂ I (Jellison)	72.3 nm		
16	Thin film	Ta ₂ O ₅	56.0 nm		
17	Thin film	TiO ₂ I (Jellison)	72.3 nm		
18	Thin film	Ta ₂ O ₅	56.0 nm		
19	Thin film	TiO ₂ I (Jellison)	72.3 nm		
20	Thin film	Ta ₂ O ₅	56.0 nm		
21	Thin film	TiO ₂ I (Jellison)	72.3 nm		
22	Thin film	Ta ₂ O ₅	56.0 nm		
23	Thin film	TiO ₂ I (Jellison)	72.3 nm		
24	Thin film	Ta ₂ O ₅	56.0 nm		
25	Thin film	TiO ₂ I (Jellison)	72.3 nm		
26	Thin film	Ta ₂ O ₅	56.0 nm		
27	Thin film	TiO ₂ I (Jellison)	72.3 nm		
28	Thin film	Ta ₂ O ₅	56.0 nm		
29	Thin film	TiO ₂ I (Jellison)	72.3 nm		
30	Thin film	Ta ₂ O ₅	56.0 nm		

The computed spectrum is the same, so far. Now open the list of fit parameters in the treeview and drag the layer stack object into the list of fit parameters. The behavior of this action has been changed with object generation 4.01: Dragging an object into the list of fit parameters used to select all the object's parameters as fit parameters. In the case of layers, both the thickness and the thickness fluctuations had been selected. In most cases, however, only the thickness values of the thin films are wanted as fit parameters, like in our case here. The new property of the drag and drop action just does what is wanted in most cases: The thickness values of all thin films are selected as fit parameters - and nothing else:

Fit parameters									
File	Update	New	Slider	Fit on grid	Limits from sliders	Honey mode mobility	Delete	Delete all	Actions
Value	Name	Variation	Low limit	High limit	Factor	Digits			
63.2	Stack 1 Layer 2 SiO2 (MIR-VUV): Layer thickness	Downhill simplex	0.0	0.0	1.0000	1			
86.0	Stack 1 Layer 3 Ta2O5: Layer thickness	Downhill simplex	0.0	0.0	1.0000	1			
56.0	Stack 1 Layer 4 Ta2O5: Layer thickness	Downhill simplex	0.0	0.0	1.0000	1			
72.3	Stack 1 Layer 5 TiO2 I (Jellison): Layer thickness	Downhill simplex	0.0	0.0	1.0000	1			
56.0	Stack 1 Layer 6 Ta2O5: Layer thickness	Downhill simplex	0.0	0.0	1.0000	1			
72.3	Stack 1 Layer 7 TiO2 I (Jellison): Layer thickness	Downhill simplex	0.0	0.0	1.0000	1			
56.0	Stack 1 Layer 8 Ta2O5: Layer thickness	Downhill simplex	0.0	0.0	1.0000	1			
72.3	Stack 1 Layer 9 TiO2 I (Jellison): Layer thickness	Downhill simplex	0.0	0.0	1.0000	1			
56.0	Stack 1 Layer 10 Ta2O5: Layer thickness	Downhill simplex	0.0	0.0	1.0000	1			
72.3	Stack 1 Layer 11 TiO2 I (Jellison): Layer thickness	Downhill simplex	0.0	0.0	1.0000	1			
56.0	Stack 1 Layer 12 Ta2O5: Layer thickness	Downhill simplex	0.0	0.0	1.0000	1			
72.3	Stack 1 Layer 13 TiO2 I (Jellison): Layer thickness	Downhill simplex	0.0	0.0	1.0000	1			
56.0	Stack 1 Layer 14 Ta2O5: Layer thickness	Downhill simplex	0.0	0.0	1.0000	1			
72.3	Stack 1 Layer 15 TiO2 I (Jellison): Layer thickness	Downhill simplex	0.0	0.0	1.0000	1			
56.0	Stack 1 Layer 16 Ta2O5: Layer thickness	Downhill simplex	0.0	0.0	1.0000	1			
72.3	Stack 1 Layer 17 TiO2 I (Jellison): Layer thickness	Downhill simplex	0.0	0.0	1.0000	1			
56.0	Stack 1 Layer 18 Ta2O5: Layer thickness	Downhill simplex	0.0	0.0	1.0000	1			
72.3	Stack 1 Layer 19 TiO2 I (Jellison): Layer thickness	Downhill simplex	0.0	0.0	1.0000	1			
56.0	Stack 1 Layer 20 Ta2O5: Layer thickness	Downhill simplex	0.0	0.0	1.0000	1			
72.3	Stack 1 Layer 21 TiO2 I (Jellison): Layer thickness	Downhill simplex	0.0	0.0	1.0000	1			
56.0	Stack 1 Layer 22 Ta2O5: Layer thickness	Downhill simplex	0.0	0.0	1.0000	1			
72.3	Stack 1 Layer 23 TiO2 I (Jellison): Layer thickness	Downhill simplex	0.0	0.0	1.0000	1			
56.0	Stack 1 Layer 24 Ta2O5: Layer thickness	Downhill simplex	0.0	0.0	1.0000	1			
72.3	Stack 1 Layer 25 TiO2 I (Jellison): Layer thickness	Downhill simplex	0.0	0.0	1.0000	1			
56.0	Stack 1 Layer 26 Ta2O5: Layer thickness	Downhill simplex	0.0	0.0	1.0000	1			
72.3	Stack 1 Layer 27 TiO2 I (Jellison): Layer thickness	Downhill simplex	0.0	0.0	1.0000	1			
56.0	Stack 1 Layer 28 Ta2O5: Layer thickness	Downhill simplex	0.0	0.0	1.0000	1			
72.3	Stack 1 Layer 29 TiO2 I (Jellison): Layer thickness	Downhill simplex	0.0	0.0	1.0000	1			
56.0	Stack 1 Layer 30 Ta2O5: Layer thickness	Downhill simplex	0.0	0.0	1.0000	1			
72.3	Stack 1 Layer 31 TiO2 I (Jellison): Layer thickness	Downhill simplex	0.0	0.0	1.0000	1			

The only thing to do now is to press F7 and then 'Start' in the main menu (or just 'f' on your keyboard) to start the automatic downhill simplex fit. After a while the quality of the edge filter is improving a lot. It may look like this:



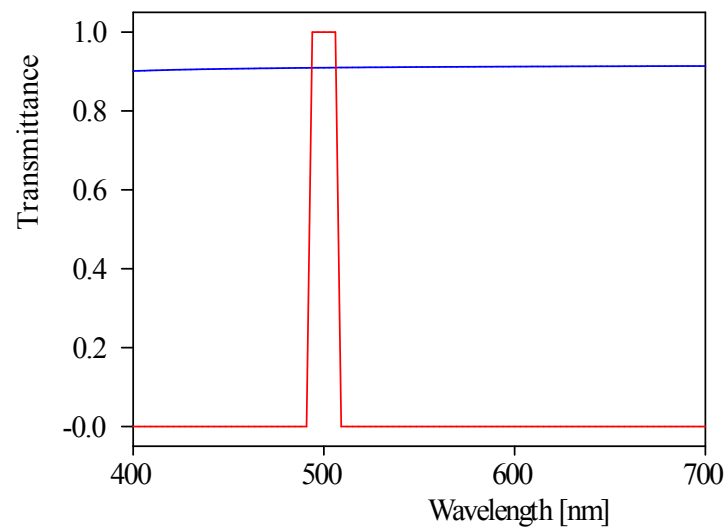
Please note that the main loss in transmission on the left side is due to the backside reflection of the glass substrate. That could be avoided with a rather simple anti-reflection coating on the backside.

5.2 Bandpass filters

Bandpass filters can be made by Fabry-Perot resonators, i.e. two Bragg filters enclosing a cavity. Therefore the following layer stack has been tried:

Thin film	Vacuum			50.0 nm
_Begin superlattice		Repeat	15 times	
Thin film	Vacuum			50.0 nm
Thin film	Vacuum			50.0 nm
_End superlattice				
Thin film	Vacuum			50.0 nm
_Begin superlattice		Repeat	15 times	
Thin film	Vacuum			50.0 nm
Thin film	Vacuum			50.0 nm
_End superlattice				
Thin film	Vacuum			50.0 nm
Thick layer	Glass (microscope slide), Vis			1.000 mm

The target spectrum is shown in red in the graph below:

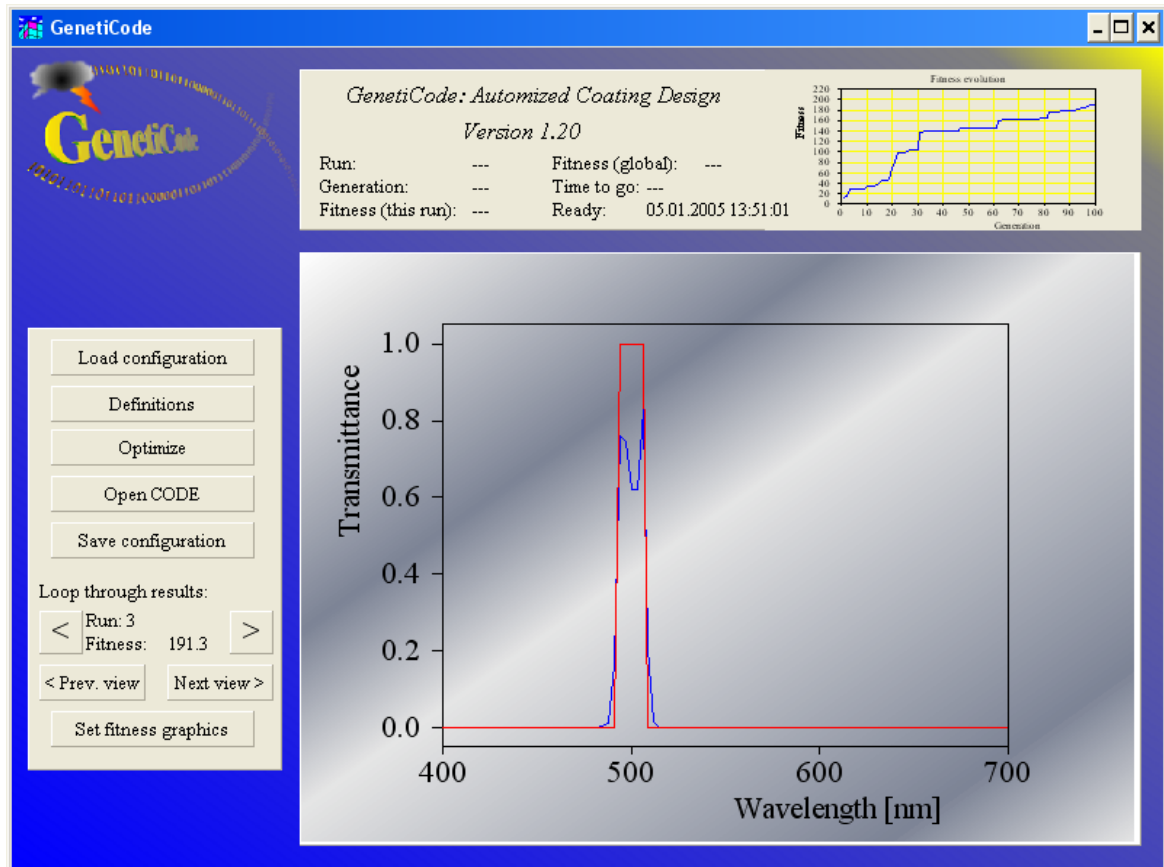


Again only SiO₂, Si₄N₃, Ta₂O₅ and TiO₂ are possible materials.

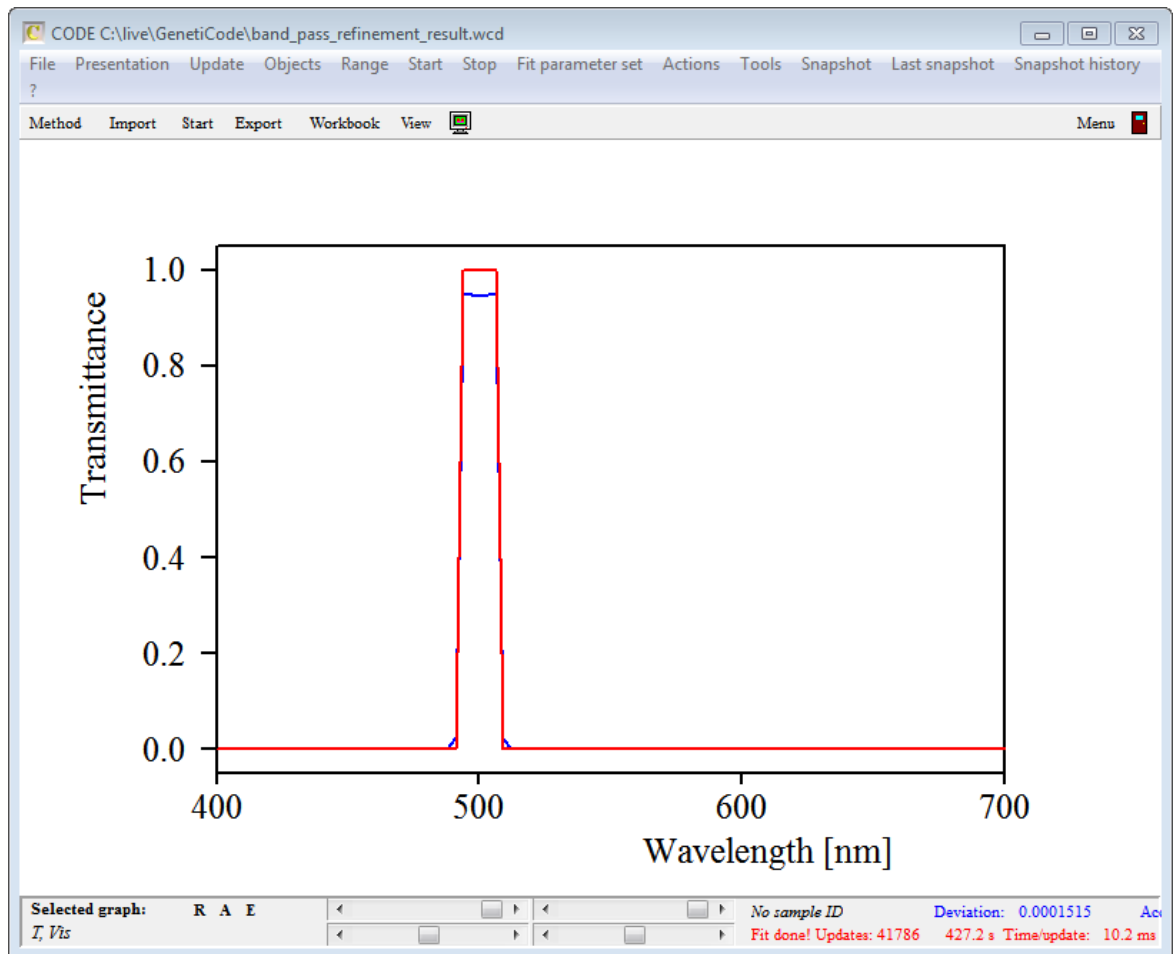
Four runs have been processed with the following parameters and fitness results:

Workbook					
File Copy Paste Clear Graph Autosize cells Test					
A25					
	A	B	C	D	E
1	Genetic algorithm parameters				
2					
3	Run	1	2	3	4
4	Fitness	103.9919464	78.4034826	191.2724734	161.6556244
5	Population	200	1000	1000	1000
6	Generations	20	50	100	100
7	Crossover probability	0.7	0.7	0.7	0.7
8	Mutation probability	0.5	0.8	0.8	0.8
9					
10					

Run 3 is the most successful:



Using this solution as starting point, one can do the manual refinement as discussed for the edge filter also here. The best result is this:

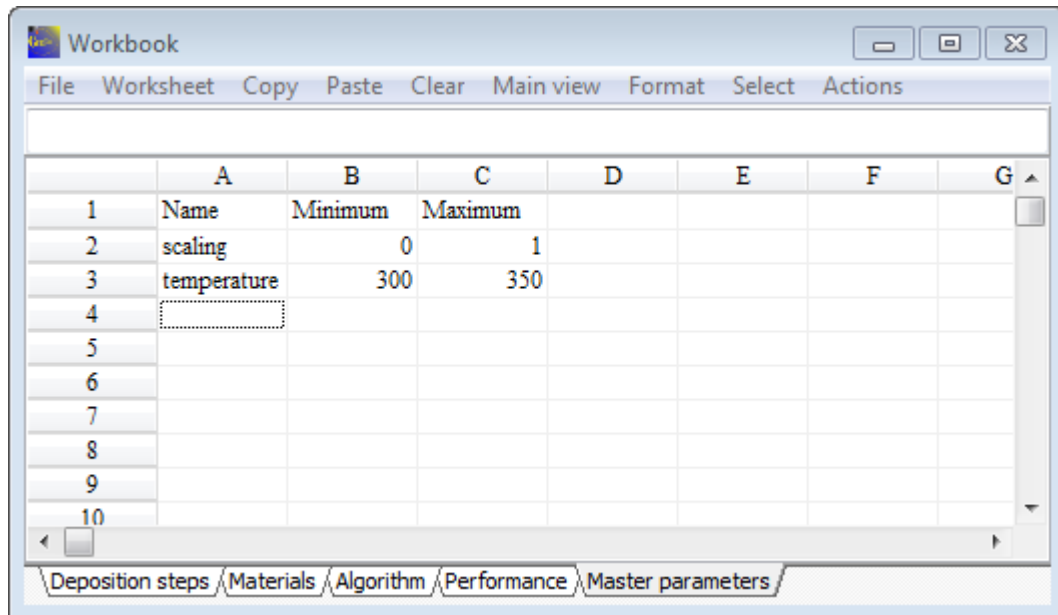


Again, the loss in transmission is due to the backside reflection. In this case the transmission can be raised to almost 100% with a very simple AR coating on the glass backside.

6 Master parameters

It might be useful for advanced coating design goals to connect model parameters by master parameters. If you would like to let GenetiCode find the best value of one or more master parameters you have to add a new worksheet called 'Master parameters' to the 'Definitions' workbook.

The structure of the 'Master parameters' worksheet is very simple: The first row must contain 3 column labels 'Name', 'Minimum' and 'Maximum'. Starting with row 2 you can enter name, wanted minimum and maximum value of each master parameter you want to optimize. Please note that the name of a parameter must exactly agree with the name used in the underlying CODE configuration. Here is an example of a worksheet setting parameters for 2 master parameters:



	A	B	C	D	E	F	G
1	Name	Minimum	Maximum				
2	scaling	0	1				
3	temperature	300	350				
4							
5							
6							
7							
8							
9							
10							